

# **Supporting Information**

## **Conformational Analysis of Olefin-Carbene Ru Metathesis Catalysts**

**Diego Benitez, Ekaterina Tkatchouk and William A. Goddard, III**

Contribution from the Materials and Process Simulation Center, Beckman Institute (139-74), Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125

[wag@wag.caltech.edu](mailto:wag@wag.caltech.edu)

**Computational Methods.** Calculations were performed on all systems using density functional theory (DFT) with the B3LYP, M06 and M06-L functionals, as implemented in Jaguar 7.0 (release 207).<sup>1</sup> B3LYP utilizes both exact Hartree-Fock (HF) exchange and corrections (generalized gradient approximation) to the Slater exchange functional, the Becke three-parameter functional (B3) with the Becke gradient correction,<sup>2</sup> the Vosko-Wilk-Nusair exchange functional,<sup>3</sup> and the correlation functional of Lee, Yang, and Parr (LYP).<sup>4</sup>

All calculations used the Hay and Wadt small core-valence relativistic effective-core-potential<sup>5</sup> (ECP) to describe the 1s-3d core electrons of the ruthenium atom, leaving the outer 16 electrons (4s, 4p, 4d, 5s, *etc.*) to be treated explicitly.

Our previous results showed that the LACVP\*\* basis set produces geometries in good agreement with experiment and that the extended LACV3P++\*\* basis set<sup>6</sup> describes properly the energy of intermediates relevant to olefin metathesis. Here LACVP\*\* was used for all geometry optimizations and LACV3P++\*\*(2f) for energies. LACV3P++\*\*(2f) utilizes the LACV3P++\*\* basis set as implemented in Jaguar plus a double-zeta f-shell with exponents reported by Martin and Sundermann.<sup>7</sup> All electrons were described for all other atoms using the 6-31G\*\* or 6-311++G\*\* basis sets.<sup>8</sup>

Every structure was optimized in the gas phase with the B3LYP and M06-L functionals as noted. For each B3LYP optimized structure, the analytic Hessian was calculated to obtain the vibrational frequencies, which in turn were used to obtain the zero point energies and free energy corrections (without translational or rotational components) to 298 K or as noted. Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for CH<sub>2</sub>Cl<sub>2</sub> ( $\epsilon = 8.93$  and  $R_0 = 2.33$  Å) or benzene ( $\epsilon = 2.284$  and  $R_0 = 2.60$  Å) using the PBF<sup>9</sup> module in Jaguar, which has been shown<sup>10</sup> recently to give quite accurate results. ( $\epsilon$  is dielectric constant and  $R_0$  is the solvent's probe radius, see ref. 9 for more details).

**Norbornene Ring-Opening Reaction.** All structures were optimized with the M06-L functional in the gas phase and electronic energies were obtained using the M06 functional with the LACV3P++\*\*(2f) basis set. Transition structures were located using B3LYP transition structures as initial geometries.

#### References

- (1) Jaguar 7.0 Release 207, Schrodinger, LLC, New York, NY, **2006**. See for example: Greeley, B. H.; Russo, T. V.; Mainz, D. T.; Friesner, R. A.; Langlois, J. M.; Goddard, W. A., III; Donnelly, R. E.; and Ringnalda, M. N. *J. Chem. Phys.* **1994**, *101*, 4028–4041.
- (2) (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100.
- (3) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200–1211.
- (4) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.
- (5) (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299–310 (b) Melius, C. F.; Goddard, W. A., III. *Phys. Rev. A* **1974**, *10*, 1541. (c) Melius, C. F.; Olafson, B. O.; Goddard, W. A., III. *Chem. Phys. Lett.* **1974**, *28*, 457.
- (6) The LACV3P basis set is a triple-zeta contraction of the LACVP basis set developed and tested at Schrödinger, Inc.
- (7) Martin, J. M. L.; Sundermann, A. *J. Chem. Phys.* **2001**, *114*, 3408–3420.
- (8) (a) Hariharan, P. C.; Pople, J. A. *Chem. Phys. Lett.* **1972**, *16*, 217–219. (b) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. von R. *J. Comput. Chem.* **1983**, *4*, 294. (c) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650. (d) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* **1980**, *72*, 5639. (e) Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265.
- (9) (a) Tannor, D. J.; Marten, B.; Murphy, R.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Ringnalda, M.; Goddard, W. A., III; Honig, B. *J. Am. Chem. Soc.* **1994**, *116*, 11875. (b) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. *J. Phys. Chem.* **1996**, *100*, 11775.
- (10) Bryantsev, V. S.; Diallo, M. S.; Goddard, W. A. *J. Phys. Chem. A* **2007**, *111*, 4422–4430.

## 1 M06-L

P1	0.1560755446	0.8370779360	-0.1203195191
C2	-1.3849993885	0.2982667299	0.7902340281
C3	-2.6455404477	0.5507427756	2.9468901346
C4	-3.8574883414	-0.1589105941	0.8636888677
C5	-3.9631895805	0.6084626510	2.1795368135
C6	-2.6989665124	0.3509741098	0.0045836586
C7	-1.5064627564	1.1028737815	2.0932946129
C8	-0.0246067801	0.1483240337	-1.8482710634
C9	-1.0372507447	0.4913882035	-4.1396413494
C10	1.1067952351	-0.7859470995	-3.9115675606
C11	0.2894290272	0.1403591064	-4.8051518509
C12	1.3144560197	-0.1986037593	-2.5157979585
C13	-0.8130900462	1.0989824025	-2.7578262432
C14	1.3875200252	-0.2781852212	0.7542800474
C15	1.9949995894	-2.5669347308	1.6164711382
C16	3.7408240018	-0.7595777451	1.4944677489
C17	3.4777675873	-2.2615258543	1.4233584887
C18	2.8736228164	0.0094330344	0.4982126386
C19	1.1297860373	-1.7894576740	0.6228728339
H20	-1.2245857649	-0.735407891	1.0739735273
H21	-2.4205029990	-0.4954182523	3.2102859917
H22	-2.7164441912	1.1022348131	3.8906504279
H23	-3.7046304885	-1.2275544625	1.0852861602
H24	-4.7964420447	-0.0916981221	0.3005065225
H25	-4.2026538731	1.6622413034	1.9633237147
H26	-4.7875073073	0.2176114672	2.7896772022
H27	-2.8928564564	1.3868858604	-0.3064648972
H28	-2.6260065266	-0.2505799972	-0.9113987753
H29	-1.7236499626	2.1580928052	1.8406615648
H30	-0.5592364112	1.1073888342	2.6531297161
H31	-0.5995589949	-0.7888504136	-1.7342326715
H32	-1.6501360080	-0.4193527333	-4.0423498388
H33	-1.6146136242	1.1860356468	-4.7616390625
H34	0.5825354659	-1.7503763890	-3.8165331873
H35	2.0805317782	-1.0081982638	-4.3662427559
H36	0.8600063939	1.0665049661	-4.9793971769
H37	0.1276518024	-0.3163369965	-5.7895480151
H38	1.9327858492	0.7095011832	-2.5836316752
H39	1.8799390116	-0.9119667740	-1.9100295136
H40	-0.2378365348	2.0324278598	-2.8600471316
H41	-1.7610605251	1.3981600901	-2.3020031494
H42	1.2039496907	0.0036233926	1.8067167938
H43	1.6967181688	-2.2906260751	2.6396725210
H44	1.8038929568	-3.6432723875	1.5187811290
H45	3.5226948378	-0.3935501129	2.5094104824
H46	4.8014459215	-0.5457052217	1.3113911218
H47	3.7944826438	-2.6374882349	0.4376554686
H48	4.0799440491	-2.7992763499	2.1664930837
H49	3.1515242495	-0.2902739660	-0.5212100555
H50	3.0626900100	1.0814991448	0.5842025185
H51	1.3744835772	-2.1197104092	-0.3979258898
H52	0.0752115185	-2.0449284232	0.7780698958
Ru53	0.2473955623	3.3617734030	0.3336120161
C54	1.0263866018	3.7431901071	-1.3033063535
C55	2.3079835314	3.4100557379	-1.9013626802
C56	4.6788358480	2.6489251611	-3.2060784076
C57	2.3920616266	3.4109478777	-3.3117469622
C58	3.4527708882	3.0579952309	-1.1600358682
C59	4.6248630594	2.6855002755	-1.8087616488
C60	3.5595697585	3.0160182602	-3.9580062533
H61	1.5143235197	3.7054276694	-3.8876689092
H62	3.3958382505	3.0911741089	-0.0729204642
H63	5.4999523164	2.4114699910	-1.2233571508
H64	3.5993781128	2.9958316472	-5.0449880161
H65	5.5935264568	2.3400379841	-3.7076149051
H66	0.3287054154	4.1993207419	-2.0275388777
Cl67	-1.9720718435	3.7580826245	-0.8178373450
Cl68	2.0073899175	2.9030373967	2.0534185592
C69	0.0024388092	5.3188889779	1.0324070977
N70	0.3828174344	6.4544873707	0.3949317103
N71	-0.7113620120	5.6908747940	2.1225076660
C72	0.0025424093	7.6737983458	1.1236019361
H73	0.8985926457	8.1437082692	1.5569728358
H74	-0.4592616536	8.3994211317	0.4450116840
C75	-0.9526750947	7.1402965720	2.1786181891
H76	-0.7507307516	7.5231552441	3.1856780901
H77	-2.0051257348	7.3498142735	1.9402219869

C78	1.3566792493	6.5657392198	-0.6424047763
C79	3.2731081720	6.8304692531	-2.6632144279
C80	2.7222916011	6.4823400773	-0.3095563173
C81	0.9331495290	6.8243631266	-1.9563405273
C82	1.9097628262	6.9473765041	-2.9497642541
C83	3.6587030235	6.6130249613	-1.3365013044
H84	1.5931819367	7.1233260974	-3.9781229242
H85	4.7181445684	6.5205156753	-1.0949121305
C86	-1.1590221610	4.8699846500	3.2069554370
C87	-2.0093430227	3.3728717567	5.4186791307
C88	-0.2771098044	4.6725376696	4.2887841362
C89	-2.4921861313	4.4262853924	3.2629041515
C90	-2.8857457781	3.6666141683	4.3706800666
C91	-0.7168983995	3.9034490301	5.3685298907
H92	-3.9128255549	3.3011725213	4.4145569059
H93	-0.0358710184	3.7332725958	6.2029424461
C94	3.1583374727	6.2142751840	1.0967694051
H95	4.2459034131	6.2797280040	1.1908330719
H96	2.8496663217	5.2107890290	1.4227448733
H97	2.7168579125	6.9210136505	1.8105407024
C98	-0.5256019536	6.9162324096	-2.2796610295
H99	-0.9862193563	7.8025264553	-1.8251334702
H100	-1.0762718802	6.0458252616	-1.8948468789
H101	-0.6872889572	6.9807862712	-3.3590646489
C102	4.3026805713	6.8880042603	-3.7509344491
H103	5.1787067712	7.4732073780	-3.4522248490
H104	3.9011553892	7.3225831381	-4.6708534265
H105	4.6617645541	5.8793034391	-3.9921722220
C106	1.0719069285	5.3224139156	4.3186738608
H107	1.7265926830	4.9164591705	3.5404297631
H108	1.5585023694	5.1623428487	5.2845205160
H109	1.0014544662	6.4059020047	4.1556239520
C110	-3.4896404614	4.8049459079	2.2132215507
H111	-3.0733651863	4.7372063130	1.2026783396
H112	-3.8365512767	5.8359288446	2.3637794638
H113	-4.3740456822	4.1629601624	2.2613162669
C114	-2.4423495745	2.5116569221	6.5673862205
H115	-1.9492615257	2.8009396015	7.5008910656
H116	-2.1886001252	1.4592014765	6.3876402746
H117	-3.5244485810	2.5574963544	6.7244179965

## 2 M06-L

N1	-0.0405461960	0.3550072729	-0.3798444702
C2	1.4198839192	0.4596124063	-0.4704799718
H3	1.7352956730	1.5008054265	-0.3585072009
C4	1.6889296095	-0.1109737551	-1.8486112421
N5	0.4857986577	-0.9231219685	-2.0899296308
H6	2.5844915344	-0.7371469712	-1.8981655725
C7	-0.7387447647	1.1362492516	0.5941533480
C8	0.5896576400	-2.1346714636	-2.8340305015
C9	0.7357519581	-4.5321862822	-4.2643245263
C10	0.7703150547	-3.3391785494	-2.1312986640
C11	0.5837890420	-2.0953935160	-4.2384445037
C12	0.6471268713	-3.3065128641	-4.9328490529
C13	0.8190788775	-4.5245266660	-2.8682608792
C14	0.9759935093	-3.3421911127	-0.6464911864
C15	0.4939264694	-0.7908561326	-4.9751679064
H16	0.6128367395	-3.2918734394	-6.0223647769
H17	0.9319828558	-5.4673086229	-2.3349160729
C18	0.7241558664	-5.8267278898	-5.0201061513
C19	-2.0871905609	2.7036119759	2.4776715319
C20	-0.9679562996	2.4976409305	0.3171620670
C21	-1.1189545091	0.5585352915	1.8140200353
C22	-1.8019206145	1.3616945215	2.7354456432
C23	-1.6436487430	3.2573496735	1.2706483819
C24	-0.5328227431	3.1054794569	-0.9816691837
C25	-0.7972429398	-0.8681875782	2.1373589940
H26	-2.1132627470	0.9217746317	0.8227371345
H27	-1.8521976525	4.3052934034	1.0558335944
C28	-2.8657484037	3.5319036066	3.4558573043
H29	1.8988659804	-2.8079035065	-0.3807490850
H30	0.1486510404	-2.8651134306	-0.1113984570
H31	1.4827326551	-0.3313375923	-5.0990849546
H32	-0.1276694075	-0.0590528813	-4.4454400091
H33	1.1783400246	-5.7262250537	-6.0104415286
H34	-0.3023288098	-6.1824981192	-5.1704563916
H35	1.2572595778	-6.6144851665	-4.4792117166
H36	0.2360457029	-1.1207538496	1.8733043612

H37	-1.4360251870	-1.5779220554	1.5969303580	H48	4.1927057853	-0.9824670579	-1.6914612430
H38	-0.9826512867	4.0921143140	-1.1200230846	H49	1.0809414227	1.1518620942	-1.7810269969
H39	-0.8333541557	2.4782955505	-1.8283980266	H50	1.6628515948	2.3504527773	-0.6395374819
H40	-2.4761216439	4.5526872466	3.5253516477	H51	0.5155715280	-1.3195604184	-0.8142232857
H41	-2.8531822975	3.0950295485	4.4585034621	H52	0.8110778700	-1.5828967418	0.8983988559
H42	-3.9161913115	3.6144892861	3.1516211450				
C43	-0.5467068468	-0.5526322273	-1.2664528955			3 M06-L	
Ru44	-2.4105322474	-1.0996222531	-1.3007575970	N1	-0.0891198230	-0.0547521642	0.1590723158
CI45	-2.4204972341	-3.2082638014	-0.1730088770	C2	1.3264154405	-0.3613526680	0.4082099497
CI46	-3.3109838409	1.0844944063	-1.4946522149	H3	1.8871160102	0.5554371574	0.6161015540
C47	-2.4551531337	-1.6899650242	-3.0485355706	C4	1.7335958705	-1.0492636117	-0.8803473895
H48	-1.6658306184	-1.4019386415	-3.7495322856	N5	0.4329879161	-1.4585061620	-1.4300359031
H49	-0.9278896241	-1.0631373637	3.2050912841	H6	2.3807577756	-1.9179940291	-0.7266322761
H50	0.5566620449	3.2352347365	-1.0365545301	C7	-0.7398226276	0.9441419187	0.9536054592
H51	0.0784447436	-0.9290528311	-5.9777849742	C8	0.3852591674	-2.2194351790	-2.6324166840
H52	1.0616566390	4.3626388884	-0.2645922318	C9	0.1346488125	-3.7385156023	-4.9677901977
H53	1.7736633340	0.6755385947	-2.6143937948	C10	0.5210865607	-3.6162572842	-2.5564333156
H54	1.8895848561	-0.1264614806	0.3356706407	C11	0.1908396395	-1.5600810247	-3.8597323326
C55	-3.5062725720	-2.5057586565	-3.6111461135	C12	0.0612405483	-2.3427132679	-5.0112695354
C56	-5.4701796786	-4.1551459757	-4.7692660844	C13	0.3897656609	-4.3533187500	-3.7373848962
C57	-4.6280435514	-2.9323569503	-2.8632389752	C14	0.7241653410	-4.2966439481	-1.2384401267
C58	-3.3987582142	-2.9283017362	-4.9549957050	C15	0.0886961710	-0.0687677830	-3.9297776343
C59	-4.3676093413	-3.7469018773	-5.5241475655	H16	-0.1108427900	-1.8451976409	-5.9660388826
C60	-5.5972652261	-3.7412763169	-3.4393985291	H17	0.4638198065	-5.4395937103	-3.6879620500
H61	-4.7250384714	-2.6357978745	-1.8199111841	C18	-0.0927362680	-4.5553892888	-6.2050321290
H62	-2.5337197075	-2.6105950346	-5.5357047523	C19	-1.7981346309	2.9870010497	2.5499521378
H63	-4.2660270922	-4.0704090229	-6.5570886129	C20	-0.6646930896	2.2778714173	0.5073462481
H64	-6.4525979675	-4.0606654972	-2.8495120553	C21	-1.2607743977	0.6231929083	2.2204414283
H65	-6.2269513216	-4.7975963173	-5.2127404253	C22	-1.7913426233	1.6614351083	2.9908412815
				C23	-1.2207139268	3.2758901787	1.3110838499
				C24	0.0420494863	2.6308173625	-0.7648544732
				C25	-1.1726933469	-0.7609166315	2.7844063730
				H26	-2.2068179614	1.4217204055	3.9696010471
				H27	-1.1802817786	4.3090953680	0.9666316027
				C28	-2.3979381059	4.0676621304	3.3985682468
				H29	1.6907891371	-4.0399625452	-0.7876553259
				H30	-0.0551023645	-3.9999486354	-0.5236634774
				H31	0.8691622847	0.4251873821	-3.3381724400
				H32	-0.8696043668	0.2900672736	-3.5292403822
				H33	0.3165546589	-4.0691045416	-7.0959828238
				H34	-1.1651666946	-4.6990260822	-6.3883730582
				H35	0.3535087541	-5.5506442785	-6.1235467751
				H36	-0.1828441571	-0.9383320791	3.2266748342
				H37	-1.3414137655	-1.5345193177	2.0286408342
				H38	0.0748234665	3.7145882759	-0.9037296068
				H39	-0.4650084902	2.1944021918	-1.6322986020
				H40	-2.1726032337	5.0645694194	3.0090571290
				H41	-2.0374426257	4.0190244688	4.4319459319
				H42	-3.4897731513	3.9702806127	3.4437893306
				C43	-0.6009074642	-0.7977953598	-0.8519185818
				Ru44	-2.6207938837	-0.9929223778	-1.1265890329
				CI45	-2.3902706965	-3.0677595238	0.3067768612
				CI46	-2.7821105136	1.2635912585	-2.1696360376
				C47	-2.6077307089	-2.1411360375	-2.5696070290
				H48	-1.9098000119	-0.9028872249	3.5801856522
				H49	1.0770479325	2.2631854973	-0.7683676407
				H50	0.1748148724	0.2819853928	-4.9617845829
				H51	0.6928658074	-5.3835796067	-1.3485855880
				H52	2.2369398327	-0.3700110442	-1.5860347517
				H53	1.4094152869	-1.0241393271	1.2826856246
				C54	-5.0350191783	-1.6913303548	-1.0936928563
				H55	-4.9545144954	-2.5265436104	-0.3955622399
				C56	-4.9097427694	-0.4137497686	-0.6083234279
				H57	-5.0816824138	0.4144270221	-1.292727640
				C58	-5.5741956054	-2.0615085522	-2.4520469113
				H59	-6.5865222319	-2.4537202785	-2.2675685650
				C60	-5.0216624189	0.9139614910	3.4553612856
				C61	-4.7224558880	-0.4243492251	3.1865240809
				C62	-4.6264447035	-0.8834457077	1.8747317341
				C63	-4.8329321320	0.0009754717	0.7991831431
				C64	-5.0861433839	1.3570960820	1.0831292874
				C65	-5.1972357003	1.8052435135	2.3952899446
				H66	-5.1079371866	1.2618377205	4.4829773736
				H67	-4.5687772106	-1.1212122075	4.0080762434
				H68	-4.3833400176	-1.9260241831	1.6767802680
				H69	-5.2165326505	2.0494448407	0.2530152872
				H70	-5.4240179363	2.8515770641	2.5897931445
				H71	-1.9437392986	-3.0126196900	-2.4615953441
P1	-0.5716291524	1.2424881522	0.7612152953				
C2	-1.3474366251	-0.0444043129	1.8862058201				
C3	-2.9697152628	-0.2773509278	3.8329870686				
C4	-2.5455819724	-2.2353587419	2.3315693529				
C5	-3.5716360307	-1.5280550675	3.2057897063				
C6	-1.9842731984	-1.2951063637	1.2677736862				
C7	-2.3843265087	0.6555697580	2.7777097703				
C8	-1.6877459909	1.1829716069	-0.7481208699				
C9	-2.7356973326	2.6211924974	-2.5561617137				
C10	-2.6691329929	0.1286976920	-2.8256478968				
C11	-2.6376168401	1.4691446151	-3.5483957531				
C12	-1.5725443065	0.0401832438	-1.7658297231				
C13	-1.6536605751	2.5309977345	-1.4848235900				
C14	1.0665256742	0.4765949605	0.2750614302				
C15	2.5995367791	-1.4555796655	-0.2994355217				
C16	3.1149298353	0.8299977067	-1.1820104175				
C17	3.1673673215	-0.6650516264	-1.4709899675				
C18	1.6903500202	1.2789639127	-0.8748360654				
C19	1.1675235196	-1.0312774905	0.0205283052				
H20	-0.5173183755	-0.3720532696	2.5362371821				
H21	-2.1702875276	-0.5743189373	4.5279537707				
H22	-3.7171653551	0.2529788090	4.4340287297				
H23	-1.7205830208	-2.6021124767	2.9606712627				
H24	-2.9846230850	-3.1199540077	1.8554294566				
H25	-4.4348424390	-1.2432886157	2.5858693695				
H26	-3.9569912975	-2.2033558681	3.9780298792				
H27	-2.8095946831	-0.9849574367	0.6084590659				
H28	-1.2710768828	-1.8340074420	0.6373321926				
H29	-3.1987086531	1.0318388778	2.1368222854				
H30	-1.9396649425	1.5395551821	3.2474392566				
H31	-2.6899468504	1.1053316376	-0.2869708486				
H32	-3.7223192590	2.5928084665	-2.0698284362				
H33	-2.6775830221	3.5849302060	-3.0750857773				
H34	-3.6480896034	0.0012265848	-2.3385411800				
H35	-2.5722173086	-0.6981713174	-3.5389802271				
H36	-1.6936415801	1.5528773700	-4.1074515435				
H37	-3.4409737040	1.5279196957	-4.2916052209				
H38	-0.5946978336	0.0941007928	-2.2659177330				
H39	-1.6088330505	-0.9352348686	-1.2740480616				
H40	-0.6670711948	2.6586019504	-1.9560434335				
H41	-1.7517986281	3.3516938453	-0.7656981265				
H42	1.6869434555	0.6803097764	1.1653234181				
H43	3.2321487992	-1.2884565017	0.5849884154				
H44	2.6344348818	-2.5322526168	-0.5025853267				
H45	3.7594367521	1.0523343159	-0.3189258767				
H46	3.5182582174	1.4037417847	-2.0242162793				
H47	2.5761240451	-0.8803910049	-2.3741791390				

C72	-3.5548898976	-2.3018199248	-3.7097679001
H73	-3.0270227694	-2.8636768767	-4.4943656611
C74	-4.7208319537	-3.1442930469	-3.1239388622
H75	-5.2711354215	-3.6187901871	-3.9466225059
H76	-4.3922970864	-3.9281187321	-2.4307219161
C77	-5.5966434077	-0.9444650158	-3.5064809964
H78	-5.7495152749	0.0507273803	-3.0790948201
H79	-6.4388155766	-1.1189172719	-4.1858939062
C80	-4.2567992205	-1.0537918175	-4.2646350401
H81	-3.6375081053	-0.1622397132	-4.1345125560
H82	-4.4286332932	-1.1839876675	-5.3388319130

TS34 M06-L

N1	0.0610047732	-0.0381059524	0.1929343586
C2	-0.0016271058	-0.2774861964	1.6407328380
H3	0.9771066068	-0.6195711293	2.0028649617
C4	-1.0756894158	-1.3551546049	1.7447974703
N5	-1.1991601501	-1.8226720040	0.3534346084
H6	-2.0408343760	-0.9572982570	2.0896753694
C7	0.6510945003	1.1276530398	-0.3977606365
C8	-2.1051727991	-2.8764486029	0.0026891100
C9	-3.8633494124	-4.9307194870	-0.6897180045
C10	-3.4124944219	-2.5531299696	-0.3906945997
C11	-1.6689133821	-4.2072911354	0.0995745075
C12	-2.5637682248	-5.2139211469	-0.2644191526
C13	-4.2718150469	-3.5989760169	-0.7312583872
C14	-3.8750497545	-1.1311986783	-0.4587017338
C15	-0.2890755244	-4.5366747345	0.5754718268
H16	-2.2301614145	-6.2498898199	-0.2150631139
H17	-5.2788951804	-3.3583646426	-1.0690940760
C18	-4.7985613524	-6.0327573159	-1.0836558835
C19	1.6739535403	3.3966656450	-1.6611328846
C20	1.9749689919	1.1073423509	-0.8588088871
C21	-0.1494331759	2.2828105269	-0.4904208048
C22	0.3798063521	3.3972044108	-1.1306951940
C23	2.4544923448	2.2555048766	-1.5014182756
C24	2.8960810847	-0.0540960740	-0.6425454004
C25	-1.5282405374	2.3176745969	0.0923860607
H26	-0.2399444071	4.2867080159	-1.2325890604
H27	3.4787159486	2.2523386251	-1.8731182071
C28	2.1979031390	4.5973223683	-2.3891142722
H29	-3.8263934562	-0.6395190500	0.5216014615
H30	-3.2667648343	-0.5292409978	-1.1455348489
H31	-0.1341672168	-4.2214180903	1.6151562768
H32	0.4683855720	-4.0314129384	-0.0340570700
H33	-5.2400590621	-6.5237461752	-0.2079173378
H34	-4.2818356764	-6.8094948848	-1.6562298615
H35	-5.6210777386	-5.6541916691	-1.6967417646
H36	-1.5001412897	2.4881316095	1.1776327853
H37	-2.0666082099	1.3838388806	-0.0894205071
H38	3.2415676808	-0.4755064563	-1.5910867699
H39	2.4159292709	-0.8764086015	-0.1123234784
H40	3.2809495034	4.5470000675	-2.5270859853
H41	1.9664994049	5.5264343175	-1.8597684587
H42	1.7457164164	4.6819681778	-3.3836795925
C43	-0.5998385208	-0.9789132638	-0.5072797835
Ru44	-0.4771556175	-1.0835828218	-2.5555811013
Cl45	-1.9756813465	0.8644132100	-2.8789863142
Cl46	1.3444710353	-2.6737607277	-2.0113441702
C47	-1.3803610312	-2.5189113744	-3.3905513878
H48	-2.1161762984	3.1237107761	-0.3508126533
H49	3.7805579499	0.2669354629	-0.0809297040
H50	-0.1099320556	-5.6136128312	0.5343072398
H51	-4.9109461063	-1.0785776721	-0.8031587204
H52	-0.7941353439	-2.1797722502	2.4058854542
H53	-0.2599546289	0.6418107363	2.1752446302
C54	-0.6434030688	-1.1124071477	-4.9063584349
C55	0.4657349437	-0.3823837522	-4.3793902247
C56	1.6950483338	-0.9532161076	-5.0524400289
C57	-2.7724849688	-2.8190933939	-3.6984849448
C58	-5.4197515477	-3.6133822162	-4.1908145351
C59	-3.8144096540	-1.8744830356	-3.6970885564
C60	-3.0878130707	-4.1672432490	-3.9640913536
C61	-4.3987334364	-4.5608070198	-4.2010554290
C62	-5.1206261879	-2.2722128405	-3.9444821096
H63	-3.5781051794	-0.8335242865	-3.4895704600
H64	-2.2867711066	-4.9046585404	-3.9592505430
H65	-4.6245400874	-5.6064677547	-4.3935304004

H66	-5.9155488466	-1.5307928370	-3.9402885152
H67	-6.4464299375	-3.9183246784	-4.3782911196
C68	-0.0540240078	-2.0670977615	-5.9264695520
H69	-0.6995631647	-2.8970631757	-6.2272092471
H70	2.6456503350	-0.7737320984	-4.5463646439
H71	0.3734664205	0.6908520020	-4.2043824502
C72	1.3028229655	-2.4109875699	-5.3138039072
H73	1.9694087924	-2.8939822573	-6.0361001330
H74	1.2508614872	-3.0131717887	-4.4075595322
C75	1.6032760505	-0.3847983173	-6.4958731508
H76	2.5208122968	-0.6192826138	-7.0448306976
H77	1.4821029556	0.7025844172	-6.5113317206
C78	0.3856130913	-1.1361604666	-7.0879555031
H79	-0.4157916473	-0.4650881954	-7.4125498634
H80	0.6713057013	-1.7421136153	-7.9533684234
H81	-1.6088853788	-0.632328106	-5.0655197980
H82	-0.7250431527	-3.3916849428	-3.5445962952

4 M06-L

N1	-0.0474488899	-0.1382405480	0.0118887429
C2	-0.1578377827	-0.0978904075	1.4768129469
H3	0.8441539399	-0.0536261735	1.9262315889
C4	-0.8896319506	-1.4010033360	1.7858744058
N5	-0.8084791803	-2.1306671130	0.5090553158
H6	-1.9442859556	-1.2463668780	2.0537455014
C7	0.3725615301	0.9846215924	-0.7694355908
C8	-1.2220419174	-3.4959673628	0.4128896873
C9	-2.0219308457	-6.1670275781	0.3152395524
C10	-2.4779316361	-3.8096553034	-0.1249992696
C11	-0.3686307130	-4.4851897395	0.9313451190
C12	-0.7865772941	-5.8112851932	0.8606561758
C13	-2.8539302979	-5.1545411312	-0.1558382154
C14	-3.3943421717	-2.7607893099	-0.6708977628
C15	0.9463952679	-4.1347312927	1.5573315428
H16	-0.1239907400	-6.5895752084	1.2383590442
H17	-3.8254686560	-5.4121193743	-0.5765198527
C18	-2.4255590708	-7.6068345135	0.2110941704
C19	1.1374870173	3.1185975544	-2.3935262449
C20	1.7059012813	1.0648760140	-1.2025265584
C21	-0.5680505028	1.9809771205	-1.0731892629
C22	-0.1616394579	3.0336336122	-1.8916822623
C23	2.0589196311	2.1382503830	-2.0220150254
C24	2.7197507210	0.0386901025	-0.8033859098
C25	-1.9596684023	1.9396039323	-0.5219095789
H26	-0.8885630353	3.8008023051	-2.1562290837
H27	3.0872642951	2.2086542306	-2.3773029617
C28	1.5256946205	4.2275170158	-3.3243956927
H29	-3.3753258353	-1.8373963311	-0.0817002769
H30	-3.1171315241	-2.4653444778	-1.6913020727
H31	0.8397337361	-3.9480370055	2.6347059197
H32	1.3900983277	-3.2491677753	1.0929181821
H33	-2.1588601417	-8.1721343823	1.1096563142
H34	-1.9200363838	-8.0975878678	-0.6301420536
H35	-3.5020897076	-7.7142329832	0.0499605825
H36	-2.0096970236	2.4328167466	0.4584538783
H37	-2.3220002354	0.9142266623	-0.4112204233
H38	3.7290811559	0.3667128222	-1.0679294175
H39	2.5363301833	-0.9313702251	-1.2834736910
H40	2.6045002777	4.4063266644	-3.3164342949
H41	1.0235203546	5.1657122561	-3.0704152839
H42	1.2459925632	3.9897156376	-4.3579160064
C43	-0.3838991550	-1.3411997546	-0.4882994790
Ru44	-0.2473402981	-1.7320752980	-2.4738916148
Cl45	-2.1890520489	-0.3124348862	-2.9835885266
Cl46	1.5872635428	-3.2274323044	-1.6817793293
C47	-0.5178140726	-3.1530315357	-3.9119099099
H48	0.2865702146	-3.8889854481	-3.8180977560
H49	-2.6560663456	2.4589983222	-1.1839800772
H50	2.7013804221	-0.1541519220	0.2761581602
H51	1.6600364527	-4.9550079775	1.4449813844
H52	-4.4245073834	-3.1262541526	-0.7078181387
H53	-0.4186493876	-1.9815936024	2.5853472303
H54	-0.7108983924	0.7929590647	1.7926493695
C55	-0.0944643245	-1.9266106306	-4.7403784463
H56	-0.9720103913	-1.4748108165	-5.2125564164
C57	0.6614923023	-0.7448931008	-3.9110492312
C58	-1.8397564324	-3.7776047128	-4.0342764835
C59	-4.2934848455	-5.1359870867	-4.1597566057

C60	-2.9644417064	-3.1684947566	-4.6135554093
C61	-1.9736333055	-5.0773978171	-3.5165498597
C62	-3.1879387838	-5.7481976275	-3.5749984748
C63	-4.1739820494	-3.8463182328	-4.6778432866
H64	-2.8961546447	-2.1498344600	-4.9834620266
H65	-1.1088094178	-5.5427065758	-3.0436439834
H66	-3.2720013146	-6.7500145339	-3.1588838412
H67	-5.0352862461	-3.3616520861	-5.1300127994
H68	-5.2454794984	-5.6587436551	-4.2108320353
C69	1.0608780423	-2.2766271867	-5.7187240869
H70	0.8628236869	-3.2136770098	-6.2489156678
H71	0.1531190655	0.2161638242	-4.0593465268
C72	2.0989118677	-0.7909434897	-4.3960022011
H73	2.8158290539	-0.3759108330	-3.6810131305
C74	2.3058600697	-2.2407248192	-4.8349335907
H75	3.2256959093	-2.3767605662	-5.4150180111
H76	2.2913080698	-2.9512545222	-4.0067908129
C77	1.2797846521	-1.0664180402	-6.6462753775
H78	1.8589832873	-1.3685069012	-7.5250413524
H79	0.3335647729	-0.6543649667	-7.0140498454
C80	2.0690786506	-0.0686388688	-5.7601234754
H81	3.0894515172	0.0769421330	-6.1326293689
H82	1.5987267593	0.9193541802	-5.6982875689

TS45 M06-L

N1	-0.8426330751	0.7108700311	0.5494226655
C2	0.5351939426	1.1927140896	0.7567666483
H3	0.6327148124	2.2082143335	0.3466493407
C4	1.3560795171	0.1759048313	-0.0218114095
N5	0.3405117296	-0.4160339010	-0.9070027525
H6	1.7918641832	-0.6041994443	0.6210434390
C7	-1.8883557317	0.9811899474	1.4922841233
C8	0.6778449641	-1.2847914240	-1.9899034104
C9	1.1342868273	-2.9697144610	-4.1722816852
C10	0.6963143350	-2.6769740857	-1.7857150982
C11	0.9734864382	-0.7155140187	-3.2381183461
C12	1.1903146936	-1.5804967284	-4.3167556019
C13	0.9145945194	-3.4975173217	-2.8950593191
C14	0.4851691527	-3.2655729706	-0.4255311313
C15	1.0509837317	0.7700925017	-3.4086774090
H16	1.3893587661	-1.1519314600	-5.2987416821
H17	0.9003422012	-4.5792678964	-2.7572413972
C18	1.2599557662	-3.8775175299	-5.3589983732
C19	-3.9284740192	1.4446614763	3.3504335590
C20	-2.8844316576	1.9230359310	1.1899896961
C21	-1.8769104340	0.2818614565	2.7156957762
C22	-2.9037179698	0.5326301695	3.6255380420
C23	-3.8944425779	2.1314046936	2.1364044480
C24	-2.8511936386	2.7314845333	-0.0716448547
C25	-0.7963003748	-0.7033925117	3.0453754421
H26	-2.9132027914	-0.0160322007	4.5675693766
H27	-4.6780170302	2.8541593768	1.9114069936
C28	-5.0334308064	1.6714492218	4.3399669436
H29	1.2575570838	-2.9352886935	0.2808813922
H30	-0.4817429196	-2.9757435209	0.0074369933
H31	1.8823626049	1.1990140327	-2.8335579615
H32	0.1256522784	1.2493481694	-3.0691491564
H33	1.6839114563	-3.3601018319	-6.2241385737
H34	0.2762117714	-4.2617857487	-5.6601542486
H35	1.8850260618	-4.7500676300	-5.1432426813
H36	0.1466743214	-0.2102219183	3.3196119778
H37	-0.5958199124	-1.3690274636	2.1986201876
H38	-3.7114240606	3.4058309981	-0.1185457337
H39	-2.8574555752	2.1140666035	-0.9788679182
H40	-5.6939116009	2.4861234497	4.0279897099
H41	-4.6440463568	1.9144009471	5.3352012998
H42	-5.6530598147	0.7732832740	4.4551548466
C43	-0.9108921933	-0.1703771787	-0.4681911340
Ru44	-2.6619966112	-1.0038990056	-1.2009077088
Cl45	-2.7737037145	-2.4507329394	0.8376404867
Cl46	-2.4184978485	0.6683366971	-3.0651598793
C47	-2.4338475400	-2.5509049620	-2.2154635176
C48	-2.5536998156	-2.8534101182	-3.6844218661
H49	-1.0907028213	-1.3320700710	3.8898058623
H50	-1.9430923359	3.3452443807	-0.1276350148
H51	1.2051278083	1.0377882259	-4.4570232440
H52	0.5186061469	-4.3580845510	-0.4625684988
H53	2.1630710434	0.6267611121	-0.6070893496

H54	0.7759720058	1.2285936606	1.8228061452
C55	-4.5772102588	-2.2239965623	-1.8746777411
C56	-4.7979000254	-0.8346421716	-1.6411240386
C57	-4.8094679769	-2.7957098791	-3.2694335176
H58	-5.8550193002	-2.5993024739	-3.5412779903
H59	-4.8514241336	-0.2149693281	-2.5403448666
H60	-1.6241368299	-2.5862085024	-4.2036481819
C61	-7.0889651562	0.9544215182	1.5005781263
C62	-6.7995757776	1.6521075216	0.3270694987
C63	-6.0106369020	1.0620866510	-0.6568163678
C64	-5.5108417548	-0.2441625749	-0.4973458201
C65	-5.7948168795	-0.9296317999	0.6978140579
C66	-6.5741167621	-0.3319050834	1.6826647748
H67	-7.7063432122	1.4105152716	2.2721900895
H68	-7.1885303010	2.6574223641	0.1774105693
H69	-5.7816815672	1.6018734405	-1.5752158847
H70	-5.3795459714	-1.9215230489	0.8583727679
H71	-6.7860726670	-0.8771231984	2.6002567226
C72	-3.8047618746	-2.1580890300	-4.2281617067
H73	-3.7541208586	-1.0695371411	-4.1686320052
H74	-3.9974744082	-2.4509627515	-5.2674051238
C75	-2.9704244145	-4.3325879049	-3.7940638941
H76	-2.3517696920	-4.9936742680	-3.1765077965
H77	-2.8758745914	-4.6708865001	-4.8330437237
C78	-4.4563360849	-4.2980830500	-3.3519431476
H79	-5.0983751115	-4.7990795311	-4.0836983379
H80	-4.6177909494	-4.8013339336	-2.3914153382
H81	-2.1996120821	-3.4296843567	-1.5855918766
H82	-4.7429695994	-2.9041433924	-1.0356236225

5 M06-L

N1	-0.0550961205	0.1599853097	-0.3171529722
C2	1.3819584518	0.3668132053	-0.5429356390
H3	1.5399434313	1.3390384684	-1.0316256716
C4	1.7343465331	-0.8027934157	-1.4454607153
N5	0.4149000795	-1.2080507306	-1.9564487237
H6	2.1939105189	-1.6407723195	-0.8986387693
C7	-0.7196714788	0.7597380776	0.8012475937
C8	0.3332872634	-2.2841021979	-2.8909106578
C9	0.1623693032	-4.3789681276	-4.7285289794
C10	0.1450046952	-3.5951980286	-2.4195420429
C11	0.4784291342	-2.0042746339	-4.2676354071
C12	0.3875135204	-3.0693151135	-5.1555098966
C13	0.0566641509	-4.6220153042	-3.3579390110
C14	-0.0031746714	-3.8784919225	-0.9581494064
C15	0.6627906029	-0.5996603063	-4.7379646076
H16	0.4775736709	-2.8636238049	-6.2218798642
H17	-0.1286510480	-5.6373659387	-3.0061387448
C18	-0.0049907546	-5.4948486894	-5.7145291927
C19	-1.9938335370	1.8434371057	3.0409191961
C20	-1.4622034814	1.9368405264	0.6563626470
C21	-0.5565538412	0.1406063278	2.0575332001
C22	-1.1987192493	0.6979161523	3.1551892684
C23	-2.1035087220	2.4466819959	1.7934058466
C24	-1.5665735527	2.6803733326	-0.6386149830
C25	0.2646701112	-1.1027336739	2.2027035291
H26	-1.0930650401	0.2144053949	4.1258026574
H27	-2.6909586634	3.3591513912	1.6920793198
C28	-2.7038511453	2.3950026572	4.2401058788
H29	0.8466145587	-3.4978328498	-0.3774265700
H30	-0.9005210541	-3.4018635208	-0.5407493364
H31	1.5734546350	-0.1414169130	-4.3331030303
H32	-0.1773308851	0.0315957142	-4.4200230246
H33	0.3006712818	-5.1976021132	-6.7213112554
H34	-1.0540523113	-5.8121187729	-5.7683682651
H35	0.5746301454	-6.3794671249	-5.4318109425
H36	1.3365933587	-0.9139631795	2.0583682683
H37	-0.0448282901	-1.8561003276	1.4714433358
H38	-2.5605403688	2.5824199723	-1.0893651929
H39	-0.8689118468	2.3145228671	-1.3933862046
H40	-3.1185396875	3.3877811355	4.0460640696
H41	-2.0361578527	2.4713403119	5.1048160464
H42	-3.5332565678	1.7450002711	4.5417156654
C43	-0.5969188228	-0.6946177563	-1.2175202862
Ru44	-2.6106732591	-0.8953956928	-1.4135183712
Cl45	-2.6927866071	-2.0405889128	0.7632918600
Cl46	-2.3828218173	0.7572828631	-3.2502872459
C47	-2.6067718944	-2.1783209736	-2.7539914486

H48	-2.1904869933	-1.8387510649	-3.7155274775	H42	-0.4573677939	-2.6181811406	1.9766923134
H49	0.1428453500	-1.5358026352	3.1985300317	H43	-2.0007895217	-3.0663393182	2.6788539913
H50	-1.3887723289	3.7481973648	-0.4751600379	C44	0.8680081272	-0.0182187247	6.7425778385
H51	0.7321952321	-0.5640084700	-5.8279696091	H45	1.3986216707	0.9400498387	6.7189498518
H52	-0.0779665955	-4.9534698660	-0.7737981835	H46	1.6158985339	-0.8166575077	6.7581962767
H53	2.4005980865	-0.5323612408	-2.2704499904	H47	0.3305210189	-0.0547265437	7.6972028438
H54	1.9280757211	0.3705833313	0.4050218239	C48	-2.5470558169	2.0083101173	3.6496143637
C55	-5.0988891606	-1.3741819772	-1.1837396998	H49	-2.1252985884	2.449881251	2.7355790908
H56	-4.9738794618	-2.0164598602	-0.3177818840	H50	-2.5605401320	2.7821660644	4.4215008667
C57	-4.8167736333	-0.0325462343	-1.2359136940	H51	-3.5858012125	1.7384587126	3.4249573266
C58	-3.1821130398	-3.5048773557	-2.8332381556	C52	0.9277568569	0.4012862966	1.8261224735
C59	-4.2812022922	-6.0634496280	-3.1718892474	H53	0.4758438263	0.7087065181	2.7782966552
C60	-3.5916772539	-4.2609232709	-1.7181067065	C54	2.3365057325	0.1191353884	1.8317616085
C61	-3.3313994551	-4.0654946004	-4.1188423378	C55	3.0908343154	-0.0213988619	3.0152652170
C62	-3.8879173973	-5.3259402613	-4.2873686572	H56	2.6005976793	0.1330799331	3.9757016529
C63	-4.1237069202	-5.5301212990	-1.8914026496	C57	4.4299085980	-0.3809891102	2.9408623750
H64	-3.4694086923	-3.8357520263	-0.7236743998	H58	5.0159824012	-0.5004752311	3.8484687384
H65	-3.0015366615	-3.4878794933	-4.9814529524	C59	5.0273645905	-0.6025249940	1.6931577816
H66	-4.0119090921	-5.7372405222	-5.2862856799	H60	6.0754894537	-0.8883315127	1.6411481243
H67	-4.4264738077	-6.1098326625	-1.0230563051	C61	4.2977202419	-0.4499505831	0.5143379564
H68	-4.7109872319	-7.0541431366	-3.2994150171	C62	2.9572994657	0.0645241086	0.5708415875
C69	-5.9970784994	-1.6790961698	-2.3548446000	Cl63	0.0468324568	-2.0054812326	-0.4433466150
H70	-6.0567299558	-2.7278412436	-2.6607976880	H64	4.7756774219	-0.6076195873	-0.4499940089
H71	-4.4992844435	0.5653250621	-0.3774433935	C65	1.5750535460	1.3990894902	-0.9339471099
C72	-5.5703622196	0.5291665262	-2.4203662388	C66	2.1223986738	0.1654450428	-0.6161692119
H73	-5.2215951398	1.4916098763	-2.7979594919	H67	1.1426172536	1.5552126978	-1.9219450866
C74	-5.5282473139	-0.6549625750	-3.3939468853	H68	2.0981161076	-0.6300124877	-1.3590751028
H75	-4.5250673006	-0.8402098983	-3.7870119184	H69	1.8007727228	2.2979075348	-0.3656234854
H76	-6.2349653715	-0.5421958833	-4.2240841505				
C77	-7.3606026197	-1.0448939441	-1.9410250778				
H78	-7.6968518852	-1.3894777383	-0.9577556327				
H79	-8.1332342692	-1.3258282796	-2.6651410029				
C80	-7.0642741506	0.4752925254	-1.9862097255				
H81	-7.2361094821	0.9714400685	-1.0254098735				
H82	-7.6897414715	0.9816491481	-2.7293658623				

#### 6a M06-L

Ru1	-0.0476030704	0.3789510386	0.2457760331
Cl2	-0.6407871161	2.7805919675	0.6604911103
N3	-2.9831392437	-0.1102524737	0.0160765858
N4	-2.4720338134	-0.4024746684	2.1188351699
C5	-1.9769464422	-0.0655860171	0.9143917245
C6	-4.2806548495	-0.4183214737	0.6285657524
H7	-4.7760008598	-1.2308077191	0.0851842168
H8	-4.9317296590	0.4665526388	0.5869085494
C9	-3.8869082072	-0.8037204234	2.0540781635
H10	-4.4689819827	-0.2810369810	2.8209159710
H11	-3.9753887299	-1.8829977704	2.2426463168
C12	-2.8055319614	0.1230514236	-1.3869361917
C13	-2.6096035341	-0.9819025618	-2.2434636327
C14	-2.2897044447	-0.7301110713	-3.5780008246
H15	-2.1057204026	-1.5768172176	-4.2390787083
C16	-2.1921289448	0.5704825654	-4.0834800899
C17	-2.5045330569	1.6337849701	-3.2348569452
H18	-2.5011756070	2.6505538918	-3.6271930250
C19	-2.8423295492	1.4372560786	-1.8896454727
C20	-2.8144911009	-2.3946791035	-1.7866853040
H21	-3.8156735902	-2.7402063423	-2.0787191840
H22	-2.7081052738	-2.5062195325	-0.7052369587
H23	-2.0862034118	-3.0658150207	-2.2483328795
C24	-1.7753848814	0.8060622280	-5.5049432477
H25	-2.0515620128	1.8063807161	-5.8497834526
H26	-2.2252148844	0.0759637392	-6.1854804834
H27	-0.6888357474	0.7118167800	-5.6174878327
C28	-3.3462483269	2.5947807643	-1.0826727108
H29	-4.3624019845	2.8477445048	-1.4129444753
H30	-2.7207543268	3.4804062640	-1.2164973268
H31	-3.3694480401	2.3866416227	-0.0114352819
C32	-1.7371209602	-0.3684472401	3.3438210631
C33	-0.9721593042	-1.4804819422	3.7289781328
C34	-0.1384982483	-1.3460114758	4.8458864462
H35	0.4903922919	-2.1888274678	5.1330068305
C36	-0.0651162430	-0.1562626196	5.5751505381
C37	-0.8893608891	0.9099661978	5.1947399614
H38	-0.8516739991	1.8429294441	5.7569545868
C39	-1.7349210990	0.8276926148	4.0850663866
C40	-0.9833061025	-2.7465845680	2.9319524782
H41	-0.4999102740	-3.5596940744	3.4799018622

#### 6b M06-L

Ru1	-0.7451894395	0.0220775348	0.0128904492
Cl2	-1.8136880648	2.2758840157	-0.1498590515
Cl3	-3.0570966709	-0.8303080565	-0.2268165215
N4	0.0096457419	-2.3410311240	-1.7123795960
N5	-0.4716232791	-3.0626035558	0.3050616327
C6	-0.2747649245	-1.9499410124	-0.4395446836
C7	-0.3313266990	-3.7605110550	-1.9031229593
H8	0.3687520121	-4.2532652779	-2.5812184865
H9	-1.3383368971	-3.8223040922	-2.3379926928
C10	-0.2952687913	-4.2934032477	-0.4822778319
H11	-1.1030231282	-4.9984425020	-0.2648362580
H12	0.6611467667	-4.7762562466	-0.2268811000
C13	0.7767938292	-1.6171187765	-2.6831656764
C14	2.0880543767	-2.0720734976	-2.9623753542
C15	2.8433009455	-1.3893870080	-3.9155656143
H16	3.8550425984	-1.7384330818	-4.1245402911
C17	2.3487415502	-0.2717240917	-4.5964759267
C18	1.0551711909	0.1539476420	-4.2938963794
H19	0.6449390758	1.0201779225	-4.8123398207
C20	0.2475214731	-0.4997112805	-3.3509452827
C21	2.7022117020	-3.2549278258	-2.2716084402
H22	3.7878274912	-3.1405948270	-2.2080036772
H23	2.5208526650	-4.1936252742	-2.8116833684
H24	2.3211005780	-3.3905713805	-1.2548335695
C25	3.1985329750	0.4346989557	-5.6106611918
H26	2.6518788764	1.2372669037	-6.1123261747
H27	3.5609670202	-0.2555691989	-6.3807779953
H28	4.0870791770	0.8791448258	-5.1471912443
C29	-1.1303467745	0.0119120797	-3.0713755324
H30	-1.5718249596	0.4546885843	-3.9691771862
H31	-1.1392465458	0.8278576355	-2.3267749349
H32	-1.8075798532	-0.7613760286	-2.6985400829
C33	-0.3981884531	-3.1283647242	1.7346766159
C34	0.8814236517	-3.1736244441	2.3319221458
C35	0.9655212317	-3.2059917050	3.7215996835
H36	1.9508983756	-3.2096742621	4.1880655903
C37	-0.1790450698	-3.1951993152	4.5289962381
C38	-1.4238641324	-3.2200564629	3.9040439869
H39	-2.3272966358	-3.2522231722	4.5130001728
C40	-1.5642269809	-3.2098550827	2.5079742221
C41	2.1360591632	-3.1976663064	1.5108915157
H42	2.2967766325	-4.17787920	1.0366679201
H43	3.0127182519	-2.9925684565	2.1309700659
H44	2.1187180156	-2.4530735468	0.7088244048
C45	-0.0520058253	-3.1406531869	6.0213900985
H46	0.3526616096	-2.1726998630	6.3423913722
H47	0.6334535436	-3.9063818345	6.4001268883
H48	-1.0169633326	-3.2753946950	6.5173469484

C49	-2.9335236976	-3.3044786121	1.9143082813	C56	0.8468915001	-0.3387965785	4.0644166325
H50	-3.4746539131	-2.3584616316	2.0122657687	C57	1.7895612905	0.5579377656	1.9949004084
H51	-3.5132330560	-4.0801231705	2.4257259739	C58	2.0632387779	-0.1154247637	4.7004808039
H52	-2.9134084394	-3.5130535491	0.8432084862	C59	3.0001280333	0.7883029001	2.6452339112
C53	-0.6542331933	0.0088943209	1.8649239034	C60	3.1367468252	0.4366446835	3.9914552461
H54	-1.6001124542	0.0057366104	2.4244229944	H61	4.0854095711	0.6049728850	4.4964110588
C55	0.5926823948	0.1178308748	2.5710800058	H62	0.0074936709	-0.7799545418	4.5981692366
C56	0.7284545792	0.1932541495	3.9708459612	H63	2.1830396091	-0.3694121748	5.7511990582
C57	1.7410584575	0.0973925623	1.7445374622	H64	3.8312268375	1.2401637097	2.1082362633
C58	1.9986498813	0.1978142992	4.5376751726	C65	1.6221804953	0.1778526699	-0.5323620564
C59	3.0080451856	0.0721260469	2.3261952815	C66	1.4653345349	0.9622774334	0.6119860372
C60	3.1318075049	0.1217847553	3.7170639507	H67	1.6208280317	0.6615902299	-1.5092413750
H61	4.1221293737	0.1128085448	4.1671983250	H68	1.3012159062	2.0307283430	0.4625783586
H62	-0.1633519658	0.2227201647	4.5941912871	H69	2.1237666514	-0.7878604484	-0.4943780483
H63	2.1160272828	0.2486394445	5.6173910583				
H64	3.8957440181	0.0291108555	1.6972537137				
C65	0.9793095550	1.2619206504	-0.3465075754	Ru1	-0.0724071851	-0.1490191675	0.0150657773
C66	1.4768537053	0.1071808258	0.2922702432	Cl2	0.1077846817	2.3090604852	-0.1650165930
H67	1.1194602049	1.3705928653	-1.4226043977	N3	-2.9832455625	-0.2801850058	0.0059597826
H68	2.0302816077	-0.6064575562	-0.3232525399	N4	-2.4282775427	-0.4843067258	2.1059930323
H69	0.8335649404	2.1883346893	0.2028480622	C5	-1.9382328033	-0.2501050445	0.8693328982

#### 7a M06-L

Ru1	-0.5128409668	0.0724822584	0.0699625243	H8	-5.0572215815	-0.0007130947	0.3382660714
Cl2	-1.0085385284	2.4033351110	-0.4896489734	C9	-3.8988260337	-0.5615196288	2.1245950119
Cl3	-2.9431030494	-0.3706194776	-0.0052673292	H10	-4.3102797665	0.3443352431	2.5961238790
N4	-0.2459232827	-2.2872965361	-1.7473575331	H11	-4.2306977209	-1.4243208411	2.7123776664
N5	-0.6221393732	-3.0526393647	0.2697896744	C12	-2.9044583460	0.1551476268	-1.3544971734
C6	-0.3697657589	-1.9275112340	-0.4404200919	C13	-2.7949706908	-0.7704267947	-2.4062459045
C7	-0.6793465305	-3.6762873652	-1.9612130796	C14	-2.6869485625	-0.2664891394	-3.7095929244
H8	-0.0548492884	-4.1701234536	-2.7099514223	H15	-2.5846723869	-0.9730359262	-4.5332580014
H9	-1.7178216937	-3.6733286645	-2.3215175568	C16	-2.7293429056	1.1010881890	-3.9825836524
C10	-0.5594421511	-4.2616714146	-0.5704078373	C17	-2.9239673348	1.9888892142	-2.9157025767
H11	-1.3723186640	-4.9470527530	-0.3145622052	H18	-3.0024835201	3.0574977619	-3.1143803433
H12	0.3962618246	-4.7839610357	-0.3996670875	C19	-3.0277178190	1.5406777720	-1.6004879258
C13	0.4824209668	-1.5938334755	-2.7680041080	C20	-2.8848094680	-2.2483705032	-2.1869498099
C14	1.8050863539	-2.0216768425	-3.0229936070	H21	-3.9126780997	-2.5919131900	-2.3631276126
C15	2.5426522060	-1.3562369297	-3.9995371129	H22	-2.5851930420	-2.5407060730	-1.1787290658
H16	3.5689316129	-1.6713850451	-4.1894172960	H23	-2.2402113406	-2.7913334172	-2.8839766076
C17	2.0064542999	-0.2839976051	-4.7245881701	C24	-2.5856272597	1.6179540114	-5.3825578510
C18	0.6930436582	0.1005480761	-4.4567624865	H25	-3.3171841274	2.4035017859	-5.5992976142
H19	0.2565709125	0.9283643026	-5.0146086158	H26	-2.7110364066	0.8239591166	-6.1240372017
C20	-0.0968302713	-0.5411782357	-3.4902506435	H27	-1.5950545292	2.0602927183	-5.5397606139
C21	2.4338734556	-3.1391453868	-2.2436307258	C28	-3.2976603092	2.4928375352	-0.4763940982
H22	2.1729256532	-3.0902666652	-1.1797503679	H29	-4.1616380799	2.1773966974	0.1235576799
H23	3.5237522390	-3.104528883	-2.3232470488	H30	-3.4998581666	3.4979985182	-0.8556834092
H24	2.1218960364	-4.1303246612	-2.5993696731	H31	-2.4334943407	2.5579025676	0.1947370806
C25	2.8434985510	0.4304612003	-5.7434728834	C32	-1.7224258619	-0.3681104209	3.3387550923
H26	2.2514463174	1.1290672675	-6.3401017852	C33	-1.3417787141	-1.5449147162	4.0088428380
H27	3.3307762840	-0.2711395322	-6.4291858186	C34	-0.6439634940	-1.4183685517	5.2124301856
H28	3.6441131649	1.0055901612	-5.2640321360	H35	-0.3180436279	-2.3213727171	5.7287961110
C29	-1.4963593446	-0.0760742910	-3.2385867069	C36	-0.3299456952	-0.1646931294	5.7531629591
H30	-2.1363678252	-0.8622493597	-2.8299780270	C37	-0.7286407962	0.9803939371	5.0585166652
H31	-1.9455309597	0.3080297321	-4.1591195728	H38	-0.4690320928	1.9625308019	5.4540320021
H32	-1.5274005552	0.7502260343	-2.5120633068	C39	-1.4209004113	0.9058036015	3.8449039702
C33	-0.5996392565	-3.2359690491	1.6859107452	C40	-1.6010917164	-2.8851883588	3.3908906796
C34	0.6422639753	-3.2704215789	2.3486372274	H41	-1.1781610466	-3.6887297844	3.9993896624
C35	0.6573059488	-3.5223711652	3.7206397884	H42	-1.1642542341	-2.9469974762	2.3834032663
H36	1.6131307714	-3.5159389067	4.2444204250	H43	-2.6735430241	-3.0864084874	3.2754723813
C37	-0.5214183307	-3.7433848721	4.4399694561	C44	0.4421279114	-0.0569804488	7.0348953628
C38	-1.7339396781	-3.7327645350	3.7454027462	H45	0.8506987561	0.9483953439	7.1738553687
H39	-2.6619999395	-3.9077657970	4.2888529461	H46	1.2764577939	-0.7664615833	7.0611473160
C40	-1.8007062779	-3.5023908798	2.3667158836	H47	-0.1858594294	-0.2782614761	7.9061031033
C41	1.9213410985	-3.0054439091	1.6186396180	C48	-1.7563491729	2.1425059856	3.0721569690
H42	2.7654403675	-2.9399351173	2.3112151274	H49	-1.1044006152	2.2439435100	2.1905114585
H43	1.8711395193	-2.0585822823	1.0678156336	H50	-1.6327152170	3.0387850596	3.6854507424
H44	2.1499573779	-3.7935709952	0.8892961223	H51	-2.7859877032	2.1292344289	2.6957370751
C45	-0.4714621644	-3.9839286395	5.9186892382	C52	0.9332685038	-0.2457600863	1.5875798380
H46	0.2398215466	-3.3077239481	6.4061242965	H53	0.4685159725	-0.8170213908	2.4016750215
H47	-0.1438181580	-5.0046781314	6.1488249620	C54	2.1583159669	0.3980592662	1.9695732060
H48	-1.4494058493	-3.8411994311	6.3863426367	C55	2.3723132780	0.5453496442	3.3467013237
C49	-3.1103367927	-3.5278981762	1.6460288523	H56	1.7101646568	0.0199666576	4.0321593761
H50	-3.2628774724	-2.6052699801	1.0713994201	C57	3.3583098110	1.4098776521	3.8436339930
H51	-3.9404644144	-3.6466103122	2.3463907295	H58	3.4835527615	1.5246743170	4.9177373683
H52	-3.1624009427	-4.3598893356	0.9317767525	C59	4.1394213603	2.1375454911	2.9676913010
C53	-0.4618594310	-0.2684361440	1.9027786908	H60	4.8819274671	2.8405237319	3.3420629667
H54	-1.3880336918	-0.6036928639	2.3873398688	C61	4.0084396843	1.9789493829	1.5644106999
C55	0.7105150927	-0.0227905261	2.6998053823	C62	3.0495773910	1.0525001274	1.0537702257

#### 6c M06-L



C63	2.1333519467	-0.2710886409	-0.8688636105	C64	2.7669078904	0.2416621072	3.6254539194
H64	2.3591741103	-1.2855288013	-0.5357807671	C65	2.4362924809	-0.0245856700	1.2035196740
C65	1.2257104270	-0.1063655410	-1.8875569670	C66	2.2346304224	0.4495478665	4.9245624187
H66	1.0553609794	0.8743175497	-2.3299731521	C67	4.1620481617	0.0962325596	3.4399339979
H67	0.7985927382	-0.9773595222	-2.3835669351	C68	3.8130297154	-0.1918957220	1.0765018474
Cl68	-0.1623116823	-2.6158003102	-0.2164812513	H69	2.9290447028	0.5231717395	5.7600369866
C69	2.9899195787	0.8083352154	-0.3458708327	C70	4.6773401803	-0.1275054426	2.1813834442
C70	3.7914623711	1.5515326133	-1.1979707745	H71	4.8144736353	0.1591463360	4.3086279380
H71	3.7350684763	1.3634136300	-2.2680686142	H72	4.2252071963	-0.3610586251	0.0818672834
C72	4.6886503866	2.5179299292	-0.6993509000	H73	5.7483596640	-0.2470754473	2.0368983006
H73	5.3011023805	3.0890562977	-1.3928867681	H74	-1.0771243346	0.4577151402	4.2043603972
C74	4.8156559158	2.7117209084	0.6578433462	H75	0.4798539960	0.7132321714	6.1293078894
H75	5.5368410191	3.4229085994	1.0557951968				

#### 7b M06-L

Ru1	-0.5723932246	0.1070214508	-0.1199779252
Cl2	-1.3648660234	2.3827812191	-0.6941176201
Cl3	-3.0229327484	-0.4278073117	-0.1190954678
N4	-0.1870632102	-2.3529191644	-1.7513681028
N5	-0.5273020449	-2.9982783693	0.3196903465
C6	-0.3569142787	-1.9179059194	-0.4768497713
C7	-0.4853294705	-3.7870123448	-1.8768471024
H8	0.2341932379	-4.2796209285	-2.5376076945
H9	-1.4879372283	-3.9103024767	-2.3080710508
C10	-0.4107698420	-4.2588522611	-0.4340250448
H11	-1.2209290665	-4.9412120629	-0.1597221299
H12	0.5441595199	-4.7513889088	-0.1957405951
C13	0.4300718334	-1.6273722951	-2.8233775161
C14	1.7748605425	-1.9341835051	-3.1365440849
C15	2.3903013580	-1.2468836786	-4.1823814863
H16	3.4294105324	-1.4766192805	-4.4197707631
C17	1.7125896633	-0.2775312936	-4.9301263575
C18	0.3817464426	-0.0140983555	-4.6081930287
H19	-0.1705434330	0.7254042780	-5.1870991585
C20	-0.2874415381	-0.6761705514	-3.5691283483
C21	2.5537374419	-2.9865804708	-2.4010691921
H22	3.6077862252	-2.7037398889	-2.3132487695
H23	2.5304770975	-3.9499269628	-2.9276272405
H24	2.1727785670	-3.1650507360	-1.3916399572
C25	2.4076356387	0.4568825715	-6.0371470785
H26	1.6957960720	0.9511649767	-6.7035141330
H27	3.0273808976	-0.2140332804	-6.6409523442
H28	3.0741527544	1.2318935506	-5.6410910783
C29	-1.7212497633	-0.3506993826	-3.2954196390
H30	-2.2418700283	-0.1122590731	-4.2276907591
H31	-1.8260840013	0.5334364022	-2.6479390622
H32	-2.2517230364	-1.1606739091	-2.7896443318
C33	-0.3856828361	-3.0354470307	1.7469394577
C34	0.9097692920	-3.1118410804	2.2980042027
C35	1.0416248464	-3.1217764927	3.6873479805
H36	2.0434835197	-3.1477251869	4.1175806213
C37	-0.0708861319	-3.0925800669	4.5329682419
C38	-1.3409134273	-3.1065249154	3.9513022492
H39	-2.2214833085	-3.1327746801	4.5928082419
C40	-1.5273604337	-3.0977320107	2.5639991386
C41	2.1358128929	-3.2324298078	1.4447853650
H42	2.2994610556	-4.2715633769	1.1282260915
H43	3.0302353690	-2.9154789382	1.9889882193
H44	2.0724947604	-2.6250630621	0.5395689139
C45	0.1071261577	-3.0446429469	6.0197872480
H46	0.4505399483	-2.0510575590	6.3349315602
H47	0.8622218354	-3.7604828011	6.3613175248
H48	-0.8258151288	-3.2557824866	6.5494826636
C49	-2.8984260272	-3.1883423699	1.9769852144
H50	-3.1298815832	-2.3152313416	1.3528040100
H51	-3.6546702424	-3.2732952586	2.7611282497
H52	-2.9917887932	-4.0674413288	1.3270314362
C53	-0.5529969023	0.0823833880	1.7299852873
H54	-1.5765090425	0.0172711812	2.1300921954
C55	1.6635219402	-0.0395435804	-0.0626718276
H56	1.9714736379	-0.8429010378	-0.7342587703
C57	1.2328194109	1.1456834064	-0.6810186978
H58	1.2937834130	2.0973017245	-0.1597539320
H59	1.1819730075	1.2131726627	-1.7681400213
C60	0.4625255305	0.2428319219	2.7339196801
C61	-0.0016054365	0.4223251493	4.0419350176
C62	1.8803318264	0.1720616541	2.4970315960
C63	0.8759561547	0.5516739694	5.1298595396

#### 7c M06-L

Ru1	-0.3617218643	0.1481024124	0.0303301711
Cl2	-0.6501206635	2.5211418082	0.7070184858
Cl3	-2.8591658437	0.1477161662	-0.2332787633
N4	-0.4172723601	-1.6250491991	-2.4760404545
N5	-1.0490648378	-2.8147788586	-0.7483906668
C6	-0.5596786516	-1.6085183004	-1.1184407709
C7	-1.1586334979	-2.7602724019	-3.0521940245
H8	-0.6670736256	-3.1469675174	-3.9459577363
H9	-2.1648575940	-2.4147443939	-3.3272964696
C10	-1.1953399269	-3.7293676287	-1.8921171046
H11	-2.1320718102	-4.2891101760	-1.8195110485
H12	-0.3600052108	-4.4499503378	-1.8990334586
C13	0.4870789240	-0.8649728414	-3.2870809847
C14	1.5701079487	-1.5532270598	-3.8872019059
C15	2.4511408163	-0.8364198793	-4.6968173060
H16	3.2875497658	-1.3666258944	-5.1527768821
C17	2.3111273211	0.5388853557	-4.9111911068
C18	1.2516343595	1.1914609614	-4.2814320017
H19	1.1259668050	2.2643341894	-4.4252470578
C20	0.3267594271	0.5182117215	-3.4700525010
C21	1.8443451229	-3.0102342437	-3.6488565184
H22	1.5187572959	-3.3360324728	-2.6550273538
H23	2.9160198675	-3.2136705128	-3.7274410975
H24	1.3505687653	-3.6633474606	-4.3799582865
C25	3.2975939232	1.2761114362	-5.7674231508
H26	2.9695321672	2.2967199657	-5.9809164352
H27	3.4599753533	0.7675050181	-6.7239341288
H28	4.2768471467	1.3414594037	-5.2784825142
C29	-0.7680994297	1.2838656429	-2.7996291666
H30	-1.6529188324	0.6793616847	-2.5813412339
H31	-1.0756686373	2.1427979420	-3.4034774422
H32	-0.4417019742	1.7304510431	-1.8423582410
C33	-1.0425856499	-3.3795751386	0.5650345043
C34	0.1639010105	-3.8525486417	1.1088413722
C35	0.1429402616	-4.3840240904	2.4043793310
H36	1.0798453284	-4.7225673851	2.8466116553
C37	-1.0400871280	-4.4967032774	3.1338131646
C38	-2.2362986908	-4.0965145364	2.5247468074
H39	-3.1760343078	-4.2093761675	3.0650383473
C40	-2.2677392843	-3.5500338233	1.2417559376
C41	1.4517180058	-3.8881518258	0.3395488121
H42	1.6825124428	-4.9166122641	0.0336705935
H43	2.2935407659	-3.5478418221	0.9521385448
H44	1.4293371545	-3.2747619328	-0.5638746005
C45	-1.0442905579	-5.0156506403	4.5398438781
H46	-1.2982484844	-4.2207500112	5.2521795280
H47	-0.0687161089	-5.4164063348	4.8276224279
H48	-1.7907066829	-5.8051012711	4.6777483813
C49	-3.5635426086	-3.1618883449	0.6050047670
H50	-3.5615919823	-2.1027644000	0.3146535620
H51	-4.4015727544	-3.3400790957	1.2830508333
H52	-3.7503592022	-3.7388746972	-0.3097931362
C53	-0.4482820220	-0.6036745987	1.7143677045
H54	-1.4243634604	-1.0463974950	1.9628011092
C55	1.7025430593	0.7748462386	0.3500292920
H56	1.8618152989	1.6446713159	-0.2891119651
C57	1.7048485826	-0.4980286091	-0.2554445136
H58	1.9435725003	-1.3672264006	0.3517969035
H59	1.9280417516	-0.5969786281	-1.3165519255
C60	0.4826407656	-0.5827949002	2.8082388177
C61	0.0853405962	-1.2904319235	3.9515707310
C62	1.7052473163	0.1793384055	2.8388304864
C63	0.8568490497	-1.3068790312	5.1198239151
C64	2.4349337895	0.2313241899	4.0737967487

C65	2.1881068483	0.9406288546	1.7323063222	C72	-1.7854235648	-3.7127639134	2.3556188323
C66	2.0041755797	-0.5433481621	5.1800995505	H73	-1.5595852495	-4.2811301817	3.2666994702
C67	3.5722439673	1.0677892991	4.1943192654	H74	-2.8092406030	-3.3327219583	2.4535415459
C68	3.2712932139	1.7909683607	1.9788899969	H75	-1.7672866218	-4.4132102487	1.51218059744
H69	2.5936310421	-0.5026850612	6.0947166036	C75	-1.9139100126	2.9860733704	4.6428484671
C70	3.9648236394	1.8596048483	3.1398918191	H76	-0.9814779677	3.1221168147	4.0881200528
H71	4.1102690832	1.0837410550	5.1398706708	H77	-2.5391542217	3.8651382794	4.4555903377
H72	3.6122433262	2.3870206476	1.0745323285	H78	-1.6878178823	2.9706748613	5.7160208835
H73	4.8216761321	2.5218208112	3.2360322075	C78	-3.8986959196	1.5124796592	5.0467970032
H74	-0.8585874578	-1.8314715079	3.9111862306	H79	-3.6361543178	1.4196535597	6.1078804570
H75	0.5308518919	-1.8833418852	5.9816558245	H80	-4.5793159356	2.3650015137	4.9467757667

# 8a M06-L

Ru1	0.0042752231	0.8378698409	0.3573129464
Cl2	-1.0021671737	2.9530571625	1.2639795472
N3	-2.9068242163	0.0433757488	-0.1125973265
N4	-2.4339530842	-0.1856292461	2.0107790120
C5	-1.9107064275	0.1101064269	0.8014648692
C6	-4.2196419725	-0.0112800655	0.5497145269
H7	-4.9143750938	-0.6423202004	-0.0083851503
H8	-2.6357433520	1.0071172797	0.5977219228
C9	-3.8603359951	-0.5424370265	1.9244792293
H10	-4.4225529732	-0.0690585040	2.7353806938
H11	-3.9791548298	-1.6345067652	2.0093163639
C12	-2.7885343125	-0.1241742193	-1.5359270073
C13	-2.7755319604	-1.4417371498	-2.0561924205
C14	-2.6848067509	-1.5958138958	-3.4379689974
H15	-2.6565951110	-2.6017832470	-3.8556753165
C16	-2.5874130243	-0.5032737007	-4.3078740593
C17	-2.6031492481	0.7756349499	-3.7580853800
H18	-2.5278404195	1.6374470393	-4.4220978732
C19	-2.7029541775	0.9927739880	-2.3772438848
C20	-2.8444725294	-2.6701425580	-1.1662805366
H22	-2.5256262591	-2.3626977653	-0.1612095054
C24	-2.4269886242	-0.7191515298	-5.7834812984
H25	-2.6003948384	0.1994867290	-6.3511107933
H26	-3.1134524325	-1.4850272257	-6.1596685941
H27	-1.4130573072	-1.0630511006	-6.0205963188
C28	-2.6975241321	2.4099456667	-1.8501516603
H31	-2.6740011604	2.3740116191	-0.7536961002
C32	-1.6872816831	-0.4364189726	3.2029312789
C33	-0.8513363603	-1.5746003469	3.2705322895
C34	-0.0743493159	-1.7427081908	4.4207281577
H35	0.5981977468	-2.5979030996	4.4792872509
C36	-0.1006214814	-0.8329723618	5.4809727723
C37	-0.9549751179	0.2682048472	5.3850175126
H38	-0.9764960961	0.9935551531	6.1978890851
C39	-1.7534139429	0.4933477189	4.2589926142
C40	-0.7645218095	-2.5904322122	2.1469793807
H42	-0.9971741164	-2.0789316298	1.2057919102
C44	0.7737769666	-1.0266507286	6.6845224002
H45	1.2414933487	-0.0864305380	6.9960211434
H46	1.5702050587	-1.7512955186	6.4900312082
H47	0.2014491601	-1.3939556320	7.5446261227
C48	-2.6411389298	1.7188999322	4.1982770804
H51	-2.9296228717	1.8648967132	3.1486477184
C52	0.9073723427	0.5919174883	1.9608706853
H53	0.4203929059	0.7278440386	2.9332869162
C54	2.3184536400	0.3153013375	1.9664366979
C55	3.0085452715	-0.1530049751	3.1017367171
H56	2.4710631893	-0.2468723502	4.0449561245
C57	4.3379906362	-0.5400318366	2.9868912782
H58	4.8728195541	-0.9233719635	3.8522635831
C59	4.9879539511	-0.4553393118	1.7486962778
H60	6.0251708112	-0.7717526178	1.6632403978
C61	4.3235660079	0.0341535843	0.6233910375
C62	2.9953211398	0.4494151216	0.7293120897
Cl63	0.3389835249	-1.2034491447	-0.9782079084
H64	4.8434855325	0.1153297945	-0.3286941918
C65	1.6356867278	2.2999819322	-0.2592251745
C66	2.2303079383	1.0515017905	-0.3687752684
H67	1.2845431745	2.8114686201	-1.1509148097
H68	2.3081942013	0.5815877651	-1.3474951445
H69	1.7704052042	2.9252177369	0.6196290171
C69	0.6329306894	-3.1734158681	1.9577064904
H70	0.9277571935	-3.8294770286	2.7863001158
H71	0.6603459435	-3.7699148134	1.0399839033
H72	1.3871512280	-2.3852466157	1.8519160455

H81	-4.4490389949	0.6045781588	4.7737001368
C81	-3.9517407750	3.1656166908	-2.2865915413
H82	-4.0047575354	3.2443095800	-3.3801646611
H83	-4.8657048936	2.6646771750	-1.9489784699
H84	-3.9520487768	4.1829710341	-1.8810375521
C84	-1.4354030124	3.1452905440	-2.2978127323
H85	-1.4270342991	3.3138024082	-3.3819917928
H86	-1.3449114822	4.1135370143	-1.7948195199
H87	-0.5412211994	2.5591333124	-2.0549018180
C87	-4.2664428004	-3.2321932445	-1.0743848589
H88	-4.6022762944	-3.5865670395	-2.0566793022
H89	-4.3000260104	-4.0844095679	-0.3852777761
H90	-5.0004964121	-2.4963610402	-0.7305659038
C90	-1.8945374222	-2.7800820925	-1.6163808000
H91	-2.2256372253	-4.2422109016	-2.5543918553
H92	-0.8776947384	-3.4022453201	-1.7532541669
H93	-1.8655511540	-4.5789592087	-0.8659703896

# 8b M06-L

Ru1	-0.5593172333	0.0167361703	0.0138900914
Cl2	-1.1069518820	2.4090535127	-0.3005428741
Cl3	-2.9970837454	-0.3546777697	-0.3261295439
N4	-0.2174737589	-2.3104032299	-1.7818306981
N5	-0.5298038590	-3.1085177709	0.2432262151
C6	-0.3586434514	-1.9713408956	-0.4759151622
C7	-0.6017601765	-3.7092321837	-2.0149097403
H8	0.0753876143	-4.1831493281	-2.7320756028
H9	-1.6197637091	-3.7412688458	-2.4284651223
C10	-0.5312527080	-4.3071866254	-0.6167969706
H11	-1.3922901385	-4.9400633804	-0.3796127053
H12	0.3812458585	-4.8988548019	-0.4542868156
C13	0.4710026116	-1.5426890294	-2.7841564371
C14	1.8748030295	-1.7019934606	-2.9109115638
C15	2.5277313928	-1.0245243901	-3.9399812448
H16	3.6053232364	-1.1463107709	-4.0526032868
C17	1.8438272057	-0.1945313760	-4.8353111000
C18	0.4662368817	-0.0586767537	-4.6792824849
H19	-0.0835254900	0.5758680210	-5.3739100304
C20	-0.2478691828	-0.7286300955	-3.6764316426
C21	2.6789974917	-2.5923457957	-1.9856413107
H24	2.0524907333	-2.7857163957	-1.1079466933
C25	2.5856176527	0.5256855022	-5.9208501901
H26	1.9111113580	0.8893358412	-6.7005317663
H27	3.3334419688	-0.1197886031	-6.3935301709
H28	3.1238387892	1.3942506613	-5.5241640128
C29	-1.7547779053	-0.6130716611	-3.6389759174
H32	-2.1152339511	-1.0935596194	-2.7204372927
C33	-0.4453272568	-3.2149548445	1.6743625829
C34	0.8061484279	-3.4917151384	2.2754061337
C35	0.8879256628	-3.4630601459	3.6683726112
H36	1.8501118276	-3.6477118362	4.1462436555
C37	-0.2251757005	-3.2019059080	4.4727571343
C38	-1.4625370079	-3.0391800409	3.8492737272
H39	-2.3487222810	-2.8905406002	4.4653944438
C40	-1.6054032161	-3.0558486455	2.4571142936
C41	2.0047531799	-3.9714609275	1.4767921002
H44	1.8470262702	-3.6907037342	0.4297419351
C45	-0.0813316683	-3.0976011238	5.9604734155
H46	0.4066460265	-2.1528958131	6.2326146896
H47	0.5397757765	-3.9019827104	6.3682536040
H48	-1.0503084192	-3.1263199834	6.4664416209
C49	-2.9795538734	-3.0108907073	1.8273623374
H50	-2.8676841870	-2.6425066651	0.8015892968
C53	-0.7373745500	-0.0698830860	1.8577568776
H54	-1.7579431443	-0.049223593	2.2611687380
C55	0.3894471297	0.0138647085	2.7451395418
C56	0.3203834571	0.1642128607	4.1424349767

C57	1.6427661008	-0.0389591676	2.0974035644	H36	1.8174732843	-3.6923761967	4.1102102701
C58	1.4985659339	0.2629710207	4.8762376619	C37	-0.3076944584	-3.7569240205	4.4179672004
C59	2.8156857407	0.0574417699	2.8420317205	C38	-1.5485953280	-3.6623548545	3.7885097516
C60	2.7391793723	0.2099217574	4.2295706394	H39	-2.4526377362	-3.8025901241	4.3792956846
H61	3.6540978028	0.2934170433	4.8117546309	C40	-1.6738275679	-3.4011624497	2.4191387681
H62	-0.6506599230	0.2011217483	4.6330317510	C41	2.0709058857	-3.2924446292	1.4736199286
H63	1.4587645142	0.3870840255	5.9559061381	H42	1.8568606842	-2.8293210369	0.5014452361
H64	3.7834022115	0.0221684847	2.3437277337	C45	-0.1928681432	-4.0010744298	5.8924185458
C65	1.4418078348	0.8221271192	-0.2820850234	H46	0.1723102721	-3.1062118900	6.4120255474
C66	1.5761889458	-0.2341695556	0.6324367142	H47	0.5189839305	-4.8030154912	6.1155746659
H67	1.7027549191	0.6686093354	-1.3315097987	H48	-1.1548907689	-4.2694063136	6.3371479944
H68	1.9755199148	-1.1877896785	0.2788904003	C49	-3.0474390905	-3.3810236578	1.7855980416
H69	1.4261376015	1.8547278465	0.0556606385	H51	-2.9459819601	-2.9740375787	0.7718716200
C70	3.0056857646	-3.9483362472	-2.6165408337	C53	-0.6408043913	-0.2560518186	1.9222898836
H71	2.1122958144	-4.4796957728	-2.9610125383	H54	-1.5471043196	-0.6844063375	2.3698109713
H72	3.6654113855	-3.8259680570	-3.4838639088	C55	0.4645597712	0.0983467300	2.7725929394
H73	3.5209022404	-4.5942309993	-1.8946312118	C56	0.5734266159	-0.2272573062	4.1376490472
C73	3.9686444306	-1.9283376031	-1.5025406534	C57	1.4888314038	0.8311092079	2.1320790372
H74	4.6895977365	-1.8114383954	-2.3194846967	C58	1.7051773556	0.1624342513	4.8461630607
H75	3.7865557040	-0.9356996976	-1.0769087364	C59	2.6019551254	1.2473247009	2.8618858362
H76	4.4532674809	-2.5435598352	-0.7362432329	C60	2.7126177283	0.9009969033	4.2122824884
C76	3.3456719465	-3.3827101265	1.9041361199	H61	3.5896690437	1.2106547824	4.7760125295
H77	3.5843727687	-3.6189314423	2.9472174601	H62	-0.2224240553	-0.7955444578	4.6159824608
H78	4.1509570111	-3.8039883595	1.2907120585	H63	1.8053937131	-0.0967943587	5.8975990540
H79	3.3735653764	-2.2944641132	1.7989371862	H64	3.3863429357	1.8249356639	2.3772749954
C79	2.0756710858	-5.5022687842	1.5499378357	C65	1.5157822631	0.2126162065	-0.3228067244
H80	2.3148626117	-5.8236546203	2.5706161221	C66	1.2441371878	1.1250259795	0.7051488709
H81	1.1263419980	-5.9764598434	1.2787437147	H67	1.6160515083	0.5727374671	-1.3472077541
H82	2.8556662601	-5.8928034711	0.8857146750	H68	1.0986313236	2.1713194330	0.4350255554
C82	-3.5553825469	-4.4302176716	1.7757834926	H69	2.0201857760	-0.7291857041	-0.1081261794
H83	-2.8858584436	-5.1296447481	1.2608776706	C70	3.1640879643	-2.4614491780	2.1422576766
H84	-3.7207451728	-4.8253462779	2.7862444844	H71	3.5077880314	-2.9183470207	3.0775244216
H85	-4.5173821273	-4.4371214705	1.2520888169	H72	4.0368466686	-2.3885429671	1.4828078376
C85	-3.9519350393	-2.0731353881	2.5316935543	H73	2.8263490752	-1.4479076991	2.3728553560
H86	-4.2238646434	-2.4314873330	3.5324815012	C73	2.5892223405	-4.7147745279	1.2301175496
H87	-3.5452607983	-1.0611224477	2.6218781588	H74	2.8285832687	-5.1995486921	2.1842622393
H88	-4.8738221639	-1.9883177984	1.9490116723	H75	1.8590182961	-5.3521320180	0.7196500482
C88	-2.2211675525	0.8397850291	-3.5961060359	H76	3.5040412863	-4.7023206973	0.6266846663
H89	-1.9287847436	1.3852591207	-4.5024579005	C76	3.8129539040	-2.7155029611	-1.5959201973
H90	-3.3116644793	0.8795667388	-3.5179665949	H77	4.5474265592	-2.4593002037	-2.3675202176
H91	-1.8195264878	1.3714521012	-2.7257339100	H78	3.6813679538	-1.8307769478	-0.9631208065
C91	-2.3522161012	-1.3469804901	-4.8417002159	H79	4.2540026837	-3.5096494397	-0.9826545666
H92	-2.0359071142	-0.8795366844	-5.7830794495	C79	2.7270155458	-4.4296010338	-3.0616435005
H93	-2.0426516357	-2.3984150907	-4.8795121210	H80	3.4522292678	-4.2323097786	-3.8600908458
H94	-3.4459779674	-1.3159020859	-4.8063934316	H81	3.1275513622	-5.2424679218	-2.4447460563

# 8c M06-L

Ru1	-0.6427324483	0.1056434201	0.0981492912	H82	1.8118922973	-5.7918820197	-3.5429115430
C12	-1.3142815229	2.4025703655	-0.3690620928	C82	-1.5566616483	1.4910284624	-3.7497541266
C13	-3.0474557157	-0.5012042564	-0.1242878825	H83	-1.5829097494	1.5573861499	-4.8449560779
N4	-0.2441420364	-2.2165601922	-1.7686613164	H84	-2.5089649096	1.8694815664	-3.3678377561
N5	-0.5865814196	-3.0119897543	0.2529645740	H85	-0.7741037529	2.1590600214	-3.3758199358
C6	-0.3775847281	-1.8783356321	-0.4538505524	C85	-2.4158145779	-0.8642611091	-3.8671497275
C7	-0.6678509122	-3.6091727154	-1.9942675448	H86	-2.3256161510	-0.9052159388	-4.9599917344
H8	-0.0146619393	-4.1006904043	-2.7204814262	H87	-2.3321034235	-1.8850054309	-3.4809314990
H9	-1.6923508870	-3.6117189398	-2.3918190449	H88	-3.4154912644	-0.4983946680	-3.6141975900
C10	-0.5982684633	-4.2093927863	-0.6037842467	C88	-4.0147151780	-2.4662354956	2.5320956232
H11	-1.4636108757	-4.8340222072	-0.3604676962	H89	-4.2243966648	-2.8320515007	3.5448659337
H12	0.3123116297	-4.8033660887	-0.4320450185	H90	-3.6272279632	-1.4449455836	2.5991662126
C13	0.5519956931	-1.5559700604	-2.7739504105	H91	-4.9662702034	-2.4066629340	1.9949509388
C14	1.8495185883	-2.0582114105	-3.0213908737	C91	-3.6103303001	-4.8023660347	1.7046091764
C15	2.5989349830	-1.4858386313	-4.0529171321	H92	-3.7632272355	-5.2228510343	2.7065939492
H16	3.5971567984	-1.8752558263	-4.2569266943	H93	-4.5781002683	-4.8051020359	1.1918505282
C17	2.1194829677	-0.4231905448	-4.8175256322	H94	-2.9422964953	-5.4859104633	1.1665222545
C18	0.8440450973	0.0679784926	-4.5266836854				
H19	0.4605808975	0.9050123388	-5.1066089800				
C20	0.0370264631	-0.4797118071	-3.5244558122	Ru1	0.0919999563	0.5900839865	0.2465605511
C21	2.4921058002	-3.1750163321	-2.2179703548	C12	-0.6620346902	2.8802235488	0.8048125639
H22	1.8186119124	-3.4412457053	-1.3949522676	N3	-2.8617901814	-0.0222101056	-0.0660829664
C25	2.9633814091	0.1912409664	-5.8942916112	N4	-2.3735767874	-0.2270187818	2.0550595389
H26	2.3530212363	0.6931217767	-6.6503431104	C5	-1.8478056887	0.0299662024	0.8346070767
H27	3.5826545430	-0.5572052052	-6.3989890635	C6	-4.1872447072	-0.1816306222	0.5702281138
H28	3.6467827923	0.9433355093	-5.4821989636	H7	-4.7731914866	-0.9464390337	0.0546516571
C29	-1.3533283558	0.0605298669	-3.2728174765	H8	-4.7368079529	0.7659699859	0.5226990414
H32	-1.5345413029	0.0651514972	-2.1872306601	C9	-3.8137202258	-0.5693158119	2.0020279370
C33	-0.4980839066	-3.2092070546	1.6700647670	H10	-4.3689161611	-0.0089250447	2.7581937562
C34	0.7785532005	-3.3402980095	2.2661077698	H11	-3.9481324941	-1.6397393515	2.2021687934
C35	0.8403141531	-3.6037997640	3.6349720099	C12	-2.7807883364	0.0130875188	-1.5063329520

# 6a B3LYP

C13	-2.6996025855	-1.2166271660	-2.1978227874	C20	-0.6593952546	-1.0060594991	-3.7235233880
C14	-2.6541722009	-1.1900465322	-3.5921033596	C21	2.6890304090	-2.2637332195	-2.3075454209
H15	-2.5762586408	-2.1326688287	-4.1293694592	H22	2.8185406812	-1.8501149632	-1.3041734834
C16	-2.7178957611	0.0070347566	-4.3126507578	H23	3.6652187710	-2.2379559847	-2.7993118472
C17	-2.8797612893	1.1963316049	-3.6012098581	H24	2.4077088395	-3.3159051055	-2.1857463830
H18	-2.9869451909	2.1322487855	-4.1450374802	C25	1.6600405804	0.7276052871	-6.2314976842
C19	-2.9418297776	1.2267185145	-2.2013597648	H26	0.9396126719	0.7229680500	-7.0550761242
C20	-2.7252029505	-2.5429437968	-1.4760862316	H27	2.6207763366	0.3696944414	-6.6148114511
H21	-3.6875832589	-2.7032060350	-0.9726398462	H28	1.7979294586	1.7714170144	-5.9246008849
H22	-1.9297591651	-2.6077511416	-0.7319852918	C29	-2.1436990426	-1.2305838447	-3.5727836915
H23	-2.5890755937	-3.3639406458	-2.1850387042	H30	-2.4306233738	-2.1992595750	-4.0056331752
C24	-2.6279193016	0.0008588803	-5.8204018493	H31	-2.7018083638	-0.4594771271	-4.1096155483
H25	-3.0371475447	-0.9189021142	-6.2518174912	H32	-2.4585945242	-1.1981625172	-2.5285443291
H26	-3.1701193644	-0.8484936644	-6.2493984791	C33	-0.6415444815	-3.1806316623	1.7458410375
H27	-1.5852264261	-0.0831225572	-6.1504456984	C34	0.4880071742	-3.5961074442	2.4737630734
C28	-3.2731291840	2.5228139394	-1.5014808965	C35	0.3631915819	-3.7693489280	3.8574351246
H29	-4.3239637001	2.5249866513	-1.1814382048	H36	1.2382643549	-4.0778126499	4.4261154122
H30	-3.1436418512	3.3687709390	-2.1823518218	C37	-0.8458074856	-3.5629598570	4.5209883892
H31	-2.6499871674	2.6978484129	-0.6227959042	C38	-1.9639369609	-3.2042685742	3.7596262609
C32	-1.7007567393	-0.3912602812	3.3139134407	H39	-2.9240966110	-3.0732534719	4.2538368027
C33	-1.0974886671	-1.6247793018	3.6234486266	C40	-1.8946840875	-3.0222376147	2.3765512948
C34	-0.4930937218	-1.7655725240	4.8781443705	C41	1.8224178605	-3.9036895519	1.8302963308
H35	-0.0137130984	-2.7110619564	5.1223413771	H42	2.0850731974	-4.9583098937	1.9758444035
C36	-0.4896821658	-0.7327212200	5.8199918457	H43	2.6200480805	-3.3100427833	2.2898118751
C37	-1.1189381651	0.4709074825	5.4855692897	H44	1.8287561074	-3.7036097106	0.7579149198
H38	-1.1282779464	1.2858860409	6.2061052104	C45	-0.9476170694	-3.7125595291	6.0206700037
C39	-1.7386440159	0.6638624741	4.2467375992	H46	-0.7543404601	-2.7555857818	6.5211085510
C40	-1.0736563124	-2.7688440727	2.6383821232	H47	-0.2188078551	-4.4332971318	6.4038929328
H41	-0.6195787379	-3.6537152843	3.0921954739	H48	-1.9461333866	-4.0423178525	6.3239219019
H42	-0.5042899227	-2.5170606119	1.7374775291	C49	-3.1424325322	-2.6999998200	1.5917421360
H43	-2.0833578339	-3.0461737444	2.3134236676	H50	-3.0311820504	-1.7892890071	0.9945040187
C44	0.1470219578	-0.9191967283	7.1783312559	H51	-3.9944280760	-2.5731206450	2.2650284157
H45	0.6192877904	0.0040946001	7.5290829358	H52	-3.3948454451	-3.5114907013	0.8966013526
H46	0.9080139611	-1.7049804162	7.1599384812	C53	-0.4094951208	0.1124469138	1.8438296649
H47	0.06002963470	-1.2050282412	7.9295232645	H54	-1.4447918496	0.3008955300	2.1375724463
C48	-2.4021249367	1.9813570028	3.9235748954	C55	0.6098495036	0.0817876269	2.8687245889
H49	-1.9753178923	2.4301508632	3.0205536650	C56	0.3745555591	0.3373741435	4.2316349669
H50	-2.2798091718	2.6841305917	4.7520882916	C57	1.9104636903	-0.2202453599	2.4154567916
H51	-3.4791844784	1.8624332428	3.7514112725	C58	1.4337783053	0.2846926066	5.1342506109
C52	1.0138202361	0.4694854410	1.8465400182	C59	2.9640455278	-0.2763583815	3.3258530390
H53	0.5168432525	0.6060606338	2.8076586582	C60	2.7217283867	-0.0234951400	4.6812922245
C54	2.4403673371	0.2467207809	1.8834773921	H61	3.5461336174	-0.0617320304	5.3883542319
C55	3.1256825925	-0.0603651534	3.0769415877	H62	-0.6312073893	0.5756811182	4.5668113149
H56	2.5776668158	-0.0671697461	4.0154053976	H63	1.2632788754	0.4850538205	6.1880775240
C57	4.4743958496	-0.3911537145	3.0386130000	H64	3.9709597615	-0.5030574365	2.9849844197
H58	5.0008020050	-0.6446943664	3.9542696521	C65	2.1871666786	0.5563841548	0.0332265796
C59	5.1534589185	-0.4141618195	1.8135159861	C66	2.0375151234	-0.4691265678	0.9516471680
H60	6.2063283699	-0.6817712078	1.7859365658	H67	2.5280637697	0.3577127831	-0.9788211758
C61	4.4938204142	-0.0917097103	0.6269064845	H68	2.2945545367	-1.4840760239	0.6659484784
C62	3.1436561058	0.2638671411	0.6534746267	H69	2.2430410897	1.5888472225	0.3534591791
CI63	0.4542165221	-1.6572992657	-0.6386545694				
H64	5.0322590093	-0.1019045575	-0.3169235041			6c B3LYP	
C65	1.8038875620	1.8754936776	-0.7331868038	Ru1	-0.0742254711	0.0260875912	0.1105108045
C66	2.3936146739	0.6490040027	-0.5591379993	CI2	-0.1366044547	2.3504232123	-0.5428385879
H67	1.4029218232	2.1490901598	-1.7055845788	CI3	-2.5100692144	0.0782452761	0.0021344025
H68	2.4395204038	-0.0396546269	-1.3975573768	N4	-0.2078270513	-2.3537732981	-1.7369896167
H69	1.9125587465	2.6797326345	-0.0153911474	N5	-0.6224690220	-3.0888295893	0.2842000613
				C6	-0.2787575101	-1.9898852653	-0.4301770095
				C7	-0.6342585896	-3.7485789791	-1.9751691259
				H8	0.1045131224	-2.5875490604	-2.5875490604
				H9	-1.5922817218	-3.7605784394	-2.5071396776
				C10	-0.7413273874	-4.3057113632	-0.5530064130
				H11	-1.6923211449	-4.8085108306	-0.3623363787
				H12	0.0672977396	-5.0045722231	-0.3046221699
				C13	0.2740949662	-1.575849818	-2.8520917635
				C14	1.6280320650	-1.7064385932	-3.2266404920
				C15	2.0937905947	-0.9707147208	-4.3203713645
				H16	3.1417069524	-1.0562074625	-4.6012735650
				C17	1.2493686780	-0.1438386374	-5.0643095820
				C18	-0.1027134866	-0.0984177132	-4.7153555071
				H19	-0.7838966914	0.5060457579	-5.3092530980
				C20	-0.6221580096	-0.8141558289	-3.6319055222
				C21	2.5771053275	-2.6621231615	-2.5366497406
				H22	2.2508526689	-2.9234042931	-1.5294704317
				H23	3.5822858384	-2.2354883972	-2.4660927264
				H24	2.6662150822	-3.5950362442	-3.1084243291
				C25	1.7806846653	0.6772041627	-6.2150404577
				H26	1.0405783892	0.7708567237	-7.0158615819

H27	2.6884260149	0.2363485260	-6.6381736641	C34	-0.7040108152	-1.6271275859	5.1696344355
H28	2.0311119432	1.6926130453	-5.8847012546	H35	-0.4370109728	-2.5834204799	5.6144712188
C29	-2.1068607905	-0.7954030981	-3.3680764033	C36	-0.4436731485	-0.4455811038	5.8736388782
H30	-2.5334296124	-1.8041707778	-3.4378587241	C37	-0.7802322294	-0.7714378540	5.2743867601
H31	-2.6136832058	-0.1727901874	-4.1096053452	H38	-0.5747760880	1.6998417446	5.8026699594
H32	-2.3469685137	-0.4088787989	-2.3735515894	C39	-1.3756715912	0.8379504762	4.0087691342
C33	-0.7826389335	-3.2623332423	1.7030614446	C40	-1.5534763436	-2.9085288642	3.1648084362
C34	0.3405659590	-3.5357596410	2.5044414264	H41	-1.1812561225	-3.7594131616	3.7413885965
C35	0.1406663994	-3.7992971466	3.8653852533	H42	-1.0619004906	-2.9143452752	2.1850775230
H36	1.0075286874	-4.0066134097	4.4891794370	H43	-2.6230577685	-3.0737057367	2.9867107367
C37	-1.1316184750	-3.8077532427	4.4369817390	C44	0.1651129128	-0.4922831582	7.2564349565
C38	-2.2310116788	-3.5678962367	3.6048693422	H45	0.6010429226	-0.4712773538	7.5355554860
H39	-3.2331991895	-3.5922543871	4.0271007507	H46	0.9497201008	-1.2531791276	7.3234549317
C40	-2.0889155507	-3.3101251513	2.2401924953	H47	-0.5905184979	-0.7420944405	8.0118808779
C41	1.7499761486	-3.5414866511	1.9621701847	C48	-1.7010262858	2.1755169420	3.3889944865
H42	2.3659078630	-4.2679498579	2.5006766077	H49	-1.1201544657	2.3469773757	2.4756158729
H43	2.2177367972	-2.5588252411	2.0922696696	H50	-1.4822913442	2.9854736109	4.0898854553
H44	1.7881961659	-3.7869058033	0.8981301197	H51	-2.7594214684	2.2512325283	3.1150263660
C45	-1.3259756023	-4.0619575426	5.9133292451	C52	1.0292950078	-0.1593789895	1.5330528178
H46	-1.5096992420	-3.1243572634	6.4523941641	H53	0.5936064398	-0.7948397222	2.3069110512
H47	-0.4448441375	-4.5313566500	6.3598481706	C54	2.2572671495	-0.4746467033	1.9582407647
H48	-2.1882765225	-4.7111439927	6.0972601067	C55	2.4588296941	0.5538655284	3.3410140023
C49	-3.3135083490	-3.1076992117	1.3818385651	H56	1.7753228477	0.0269001707	4.0000050855
H50	-3.2406419915	-2.1879041531	0.7939387401	C57	3.4745370305	1.3545063672	3.8921223798
H51	-4.2093496855	-3.0481887174	2.0056453614	H58	3.5904269950	1.4122362775	4.9705256015
H52	-3.4601385681	-3.9438969886	0.6856270789	C59	4.2992921029	2.0831826910	3.0630265106
C53	-0.2179149960	-0.2415031480	1.9406681264	H60	5.0692216023	2.7277047159	3.4803869722
H54	-1.1917491941	-0.4822395267	2.3709002986	C61	4.1794773748	1.9976350676	1.6504287405
C55	0.8818186399	0.0146262623	2.8465824207	C62	3.1816218808	1.1470325238	1.0822266651
C56	0.8048450006	-0.1288324946	4.2447292311	C63	2.2570644673	-0.0438661113	-0.9405580570
C57	2.0703660081	0.4906953938	2.2504616578	H64	2.4763252824	-1.0838155201	-0.7044593204
C58	1.9032096975	0.1986392561	5.0333449791	C65	1.3539460563	0.2239736585	-1.9317253447
C59	3.1602428814	0.8321757001	3.0511269185	H66	1.1906639547	1.2407329455	-2.2748716226
C60	3.0756358390	0.6790451503	4.4377421067	H67	0.9131133120	-0.5887806266	-2.5027954864
H61	3.9260769099	0.9454388645	5.0596372599	Cl68	0.0153766686	-2.4284692073	-0.3953992198
H62	-0.1163340169	-0.4880406812	4.6947190272	C69	3.1430166745	0.9770321416	-0.3317258547
H63	1.8481000099	0.0959937149	6.1134529853	C70	4.0064567693	1.7085175059	-1.1295796295
H64	4.0682013006	1.2211338646	2.5981582207	H71	3.9744629396	1.5692286397	-2.2061504560
C65	2.1581797523	-0.3472332372	-0.1442606207	C72	4.9454366345	2.6018315814	-0.5693498363
C66	2.0290929214	0.6775317848	0.7787100045	H73	5.6054320273	3.1651489916	-1.2229009835
H67	2.3665607291	-0.0994322948	-1.1804029824	C74	5.0467022709	2.7280383665	0.7954139312
H68	2.1046890762	1.7013118346	0.4241963291	H75	5.7939080993	3.3800831319	1.2403999206
H69	2.4017484167	-1.3542766921	0.1704819112				

#### 7a B3LYP

Ru1	0.0145026729	-0.0005278161	-0.0204953214
Cl2	0.0111277459	2.4376068402	-0.0199035366
N3	-2.9587657315	-0.1104478111	0.0064213549
N4	-2.3434806830	-0.3528597543	2.0889532601
C5	-1.8816791578	-0.1418044628	0.8341653726
C6	-4.2295343209	-0.4318362143	0.6860739697
H7	-4.5852859300	-1.4186204994	0.3673855266
H8	-4.9970224584	0.3065616842	0.4371820369
C9	-3.8226781876	-0.4040884413	2.1626493900
H10	-4.1989581618	0.4804164802	2.6908668451
H11	-4.1459638462	-1.2912984046	2.7141200019
C12	-2.9552154631	0.1629659039	-1.4086960616
C13	-2.9431207808	-0.8968059438	-2.3375061944
C14	-2.9429842246	-0.5772598307	-3.7010687811
H15	-2.9114246953	-1.3893295600	-4.4242416388
C16	-3.0072303206	0.7413611052	-4.1544403748
C17	-3.1207589389	1.7625368063	-3.2054559946
H18	-3.2294479377	2.7918798356	-3.5396882803
C19	-3.1154762510	1.5013196289	-1.8340993982
C20	-3.0311915183	-2.3436628227	-1.9170955063
H21	-4.0829818284	-2.6318002778	-1.7831935419
H22	-2.4880714004	-2.5426216038	-0.9938502618
H23	-2.6134219151	-2.9956340468	-2.6886598410
C24	-2.9694456640	1.0625408618	-5.6300072690
H25	-3.6147760662	1.9135168423	-5.8711544196
H26	-3.2886902577	0.2092975948	-6.2356806093
H27	-1.9533194878	1.3282336507	-5.9468366308
C28	-3.3312771158	2.6268674934	-0.8522566173
H29	-4.1576367295	2.4075530493	-0.1656080205
H30	-3.5785047233	3.5504075143	-1.3829502221
H31	-2.4321824689	2.8067078862	-0.2567618777
C32	-1.6310787300	-0.3704679774	3.3357033331
C33	-1.3019357346	-1.6165046616	3.9061806828

#### 7b B3LYP

Ru1	0.0183604117	0.0000317532	-0.0396039023
Cl2	0.0796267304	2.4355569730	-0.0675370208
Cl3	-2.4261962981	0.1906101987	-0.1598311177
N4	-0.3642031124	-2.3787501483	-1.9150571355
N5	-0.6754115220	-3.0690495899	0.1381975003
C6	-0.2985448189	-1.9971561505	-0.6100156987
C7	-0.9845068060	-3.7082509906	-2.0979623137
H8	-0.4144472293	-4.3057081671	-2.8146038435
H9	-2.0062296894	-3.5927693510	-2.4782406428
C10	-0.9527226139	-4.2733026573	-0.6769410211
H11	-1.8985001126	-4.7311604195	-0.3769437736
H12	-0.1541213930	-5.0126274099	-0.5302862567
C13	0.0934952115	-1.6502319884	-3.0706722700
C14	1.4306778512	-1.8435085867	-3.4839181525
C15	1.8908664635	-1.1563272260	-4.6089805388
H16	2.9237406055	-1.2910624266	-4.9223682626
C17	1.0543007833	-0.3071624223	-5.3428443146
C18	-0.2804520106	-0.1966966242	-4.9505918206
H19	-0.9549166350	0.4266218728	-5.5328910098
C20	-0.7956208895	-0.8708271426	-3.8349000468
C21	2.3570393214	-2.7877148475	-2.7491886185
H22	2.5223528283	-2.4848789114	-1.7105581739
H23	3.3325835514	-2.8271658578	-3.2409195397
H24	1.9587465624	-3.8089578686	-2.7247162929
C25	1.5857255822	0.4690975026	-6.5246187649
H26	0.7973198701	0.6798050242	-7.2532375713
H27	2.3868020807	-0.0751399831	-7.0348448268
H28	1.9992091801	1.4333472220	-6.2034734014
C29	-2.2715584949	-0.7947870204	-3.5317926754
H30	-2.7712996406	-1.7299165906	-3.8184096707
H31	-2.7376472042	0.0101892529	-4.1060682686
H32	-2.4704215681	-0.6126447775	-2.4728071922
C33	-0.6588093804	-3.2360009195	1.5667848625
C34	0.5293196519	-3.6160010983	2.2186516654

C35	0.4953531851	-3.8239565649	3.6030579468	H36	0.4609623134	-5.1022567558	3.0719835150
H36	1.4160710998	-4.1036987620	4.1115129895	C37	-1.6210370911	-4.5931176689	3.2085656832
C37	-0.6792835388	-3.6896395043	4.3420929950	C38	-2.6932115657	-4.0068591186	2.5222406830
C38	-1.8569792075	-3.3697597599	3.6560648339	H39	-3.6793158168	-4.0007209696	2.9816667719
H39	-2.7905381236	-3.2932914303	4.2093475325	C40	-2.5471543757	-3.4373101110	1.2559850622
C40	-1.8783684702	-3.1514553758	2.2768157768	C41	1.1848995485	-4.2264328634	0.6700378182
C41	1.8358420531	-3.8464945953	1.4925162102	H42	1.4201429754	-5.2900398725	0.5439440721
H42	2.1744232507	-4.8796038918	1.6346608721	H43	1.9679837374	-3.8021127485	1.3077177659
H43	2.6239949609	-3.1972782565	1.8894350396	H44	1.2534794287	-3.7486932333	-0.3069262080
H44	1.7576384246	-3.6647878798	0.4199373415	C45	-1.8236068492	-5.1945027064	4.5802297938
C45	-0.6822427962	-3.8691469078	5.8422437664	H46	-2.1404570941	-4.4344720498	5.3042270203
H46	-0.4876428843	-2.9150257072	6.3481432820	H47	-0.9056677416	-5.6539146941	4.9572813088
H47	0.0920989831	-4.5715433589	6.1655713443	H48	-2.6039002264	-5.9643264426	4.5647053146
H48	-1.6486719116	-4.2365711827	6.2009764219	C49	-3.7553939107	-2.8871668100	0.5385241213
C49	-3.1844738469	-2.8536345064	1.5804365132	H50	-3.5639067351	-1.8856184837	0.1441556833
H50	-3.1204489325	-1.9510921778	0.9643413506	H51	-4.6108382313	-2.8351096778	1.2174251679
H51	-3.9845947411	-2.7174614185	2.3133150549	H52	-4.0474231002	-3.5351288318	-0.2988312275
H52	-3.4843574777	-3.6811490928	0.9239535843	C53	-0.2517299174	-0.5624636753	1.7061588117
C53	-0.1219048950	-0.2111097584	1.8064638307	H54	-1.2620406910	-0.8927246507	1.9587327994
H54	-1.1569478868	-0.3990362864	2.0986208227	C55	2.1211554353	0.4894933477	0.3464071539
C55	2.2435274291	-0.3489932666	0.3992331393	H56	2.3547850293	1.2959594697	-0.3416613193
H56	2.3101533867	-1.4272148314	0.4214073822	C57	2.0116446570	-0.7976733721	-0.1776567252
C57	2.1012690415	0.2987101623	-0.8180927455	H58	2.1220843150	-1.6628826059	0.4643145751
H58	2.2717772954	1.3668064209	-0.8894425692	H59	2.2264859555	-0.9526598292	-1.2281452408
H59	2.0739288055	-0.2486504047	-1.7525742621	C60	0.6417634253	-0.5367010209	2.8451801311
C60	0.7337483065	0.0773643978	2.9287847944	C61	0.1398209698	-1.1156012298	4.0164551056
C61	0.1117993222	0.1482644246	4.1795378167	C62	1.9133343725	0.1439652507	2.8878679498
C62	2.1208518563	0.4360755561	2.8180047578	C63	0.8355152940	-1.0596121316	5.2345811928
C63	0.7980772927	0.5946474206	5.3215895771	C64	2.5638408493	0.2807432581	4.1599978247
C64	2.7980821660	0.9428714264	3.9723933115	C65	2.5207386473	0.7552005305	1.7471572132
C65	2.8301336475	0.3311410905	1.5903726101	C66	2.0156366578	-0.3540227775	5.3058890129
C66	2.1105156490	1.0009268383	5.2138896344	C67	3.7388851693	1.0672302417	4.2801286735
C67	4.1429552140	1.3817825024	3.8608670309	C68	3.6370338233	1.5613743113	1.9268767965
C68	4.1383943010	0.7848178416	1.5226814047	H69	2.5409085678	-0.2530759631	6.2526477937
H69	2.6417321566	1.3808714845	6.0833882758	C70	4.2484589814	1.7229896413	3.1852072548
C70	4.7944248362	1.3202351199	2.6514895315	H71	4.2111189008	1.1560735964	5.2550424846
H71	4.6431340584	1.7701454506	4.7443384600	H72	4.0713466232	2.0502749050	1.0591292696
H72	4.6726985408	0.7082236647	0.5799758676	H73	5.1311978846	2.3492106194	3.2782111885
H73	5.8196159757	1.6680623961	2.5614055294	H74	-0.8277237153	-1.6072026691	3.9740147842
H74	-0.9382130746	-0.1191309751	4.2542229088	H75	0.4206609276	-1.5334110499	6.1195011740
H75	0.2829740776	0.6471800419	6.2763252613				

7c B3LYP				8a B3LYP			
Ru1	-0.0537788388	0.0523911026	-0.0239578507	Ru1	0.1796821847	0.6203822535	0.2258884514
Cl2	-0.0471785025	2.4822041015	0.0136549787	Cl2	-0.6562258286	2.8821038037	0.7489501251
Cl3	-2.5098571098	0.3123512717	-0.1274091389	N3	-2.7676279938	-0.0101973188	-0.1274689820
N4	-0.4499400775	-1.7240130068	-2.4021018896	N4	-2.2805662380	-0.2360841337	1.9957374961
N5	-1.0957189979	-2.8852274898	-0.6553677864	C5	-1.7493838519	0.0313906973	0.7765959053
C6	-0.5271846303	-1.7182239014	-1.0443242163	C6	-4.0877744282	-0.0641569341	0.5419273046
C7	-1.1728674372	-2.8625445273	-3.0050840751	H7	-4.7801002682	-0.7006251854	-0.0086846192
H8	-0.5828159390	-3.3215580904	-3.8017396978	H8	-4.5104501403	0.9464986112	0.5992623111
H9	-2.1196358395	-2.5116072864	-3.4331522591	C9	-3.7146502624	-0.6028502624	1.9137017370
C10	-1.3809901421	-3.7832707894	-1.7995241829	H10	-4.2757833913	-0.1436672462	2.7285607009
H11	-2.3981904207	-4.1757166702	-1.7346117217	H11	-3.8215861678	-1.6933096692	1.9849001209
H12	-0.6837917214	-4.6311245629	-1.7848007687	C12	-2.7261170270	-0.0129989406	-1.5751624341
C13	0.2876892251	-0.8039937677	-3.2353023802	C13	-2.6726154824	-1.2633394708	-2.2494269173
C14	1.5733212542	-1.2035455284	-3.6780847272	C14	-2.7303710651	-1.2576909241	-3.6439313607
C15	2.3177462831	-0.3190056852	-4.4575492131	H15	-2.6835228728	-2.2036301570	-4.1755269090
H16	3.3117017914	-0.6170104188	-4.7845830786	C16	-2.8595039950	-0.0802560839	-4.3850588876
C17	1.8189997886	0.9352722543	-4.8308644957	C17	-2.9624853385	1.1226513945	-3.6919528053
C18	0.5227924708	1.2661551120	-4.4429193631	H18	-3.1050502792	2.0406604360	-4.2552196823
H19	0.0997524622	2.2177893228	-4.7566152418	C19	-2.9188353920	1.1886462250	-2.2923909985
C20	-0.2739110900	0.4138187596	-3.6627945858	C20	-2.6458775294	-2.6100515803	-1.5230193927
C21	2.1435485327	-2.5729291073	-3.3753173564	H22	-2.2373375090	-2.4418750182	-0.5244340490
H22	1.9027590137	-2.9162080933	-2.3664203759	C24	-2.8951569068	-0.1232741709	-5.8945327795
H23	3.2321043407	-2.5700076652	-3.4794795707	H25	-3.3144077056	0.7963166115	-6.3129573277
H24	1.7580482202	-3.3272846878	-4.0742090247	H26	-3.4947333137	-0.9657246228	-6.2558896680
C25	2.6691560428	1.8987073630	-5.6255051412	H27	-1.8865703048	-0.2451755328	-6.3079226228
H26	2.0557366202	2.5538183147	-6.2510914338	C28	-3.1927535039	5.2295869996	-1.6166112977
H27	3.3763627780	1.3706735275	-6.2729478122	H31	-2.9081911203	2.4475602530	-0.5657285083
H28	3.2557508710	2.5424276205	-4.9579452434	C32	-1.6409149864	-0.4163301635	3.2734997330
C29	-1.6879316412	0.8373541856	-3.3532606075	C33	-1.0684831128	-1.6657276207	3.6030966321
H30	-2.3152022241	0.0060093494	-3.0325559554	C34	-0.5669449026	-1.8354784578	4.8998334441
H31	-2.1342078330	1.2996962126	-4.2398874007	H35	-0.1201693244	-2.7894847311	5.1677752766
H32	-1.7108505152	1.5688099352	-2.5395004421	C36	-0.6292426878	-0.8288556550	5.8641496254
C33	-1.2589351573	-3.4269812645	0.6697156462	C37	-1.2078417335	0.3911509882	5.5055064490
C34	-0.1780576767	-4.0645219674	1.3046734261	H38	-1.2604641200	1.1840185804	6.2473447900
C35	-0.3804028303	-4.6231482911	2.5752997169	C39	-1.7251448550	0.6260642575	4.2281030964
				C40	-1.0054779544	-2.8397808647	2.6284424840



C13	-2.5741717731	-0.0949542080	-0.0461964158	H85	-2.0263213880	1.4344537735	-2.7238535530
N4	-0.1807906017	-2.2898937177	-1.7199951697	C85	-2.6655771451	-1.5042486117	-4.5030303818
N5	-0.6415161356	-3.0560428471	0.2856905188	H86	-2.4854093216	-1.1142346985	-5.5116808916
C6	-0.2649873251	-1.9492331161	-0.4045195167	H87	-2.3124028260	-2.5419254880	-4.4866559742
C7	-0.7738762898	-3.6195218747	-1.9815983280	H88	-3.7484611422	-1.5132682709	-4.3364078798
H8	-0.1844581042	-4.1729920538	-2.7136504535	C88	-4.2698892237	-2.1440050297	2.2435391200
H9	-1.7914082501	-3.4968073758	-2.3712152201	H89	-4.6151061556	-2.5046838038	3.2195154554
C10	-0.7605203968	-4.2458050598	-0.5914294329	H90	-3.8037535989	-1.1647304604	2.3692751216
H11	-1.6715573046	-4.8004224588	-0.3624825766	H91	-5.1554358231	-2.0035491246	1.6147746449
H12	0.0988434438	-4.9100080568	-0.4354898522	C91	-4.0093045858	-4.4980097444	1.3695414843
C13	0.3744274534	-1.5235706429	-2.8154200666	H92	-4.3226478265	-4.9220243510	2.3306567937
C14	1.7410912525	-1.7207099452	-3.1496290905	H93	-4.9049742897	-4.3780814819	0.7500426509
C15	2.2661574526	-1.0031468383	-4.2269484828	H94	-3.3627062224	-5.2387599810	0.8859631348
H16	3.3112750869	-1.1370532200	-4.4925481877				
C17	1.4879242423	-0.1258592180	-4.9876520533				
C18	0.1350245091	-0.0096707887	-4.6755047134				
H19	-0.4894566099	0.6359651258	-5.2860137086				
C20	-0.4564408351	-0.7052036414	-3.6128102350				
C21	2.6285512223	-2.7520032722	-2.4468071456				
H22	2.1570767100	-3.0065598244	-1.4925999606				
C25	2.0980684155	0.6699835090	-6.1175304279				
H26	1.3752148227	0.8447736288	-6.9203908433				
H27	2.9666806573	0.1593941253	-6.5451414220				
H28	2.4362205212	1.6525665618	-5.7652445256				
C29	-1.9697761771	-0.6319715708	-3.4340905492				
H32	-2.2177238078	-1.0307259355	-2.4483935943				
C33	-0.7257946955	-3.2741687448	1.7096553758				
C34	0.4458818590	-3.5952005393	2.4356715901				
C35	0.3241645349	-3.8728296620	3.8019160751				
H36	1.2171807081	-4.1167508143	4.3714297295				
C37	-0.9075781394	-3.8685388792	4.4561705517				
C38	-2.0507250559	-3.6029566209	3.6997237706				
H39	-3.0199348563	-3.6315520177	4.1903718736				
C40	-1.9978453959	-3.3157497444	2.3321359365				
C41	1.8187868535	-3.7442532312	1.7812480894				
H42	1.7556388869	-3.3371514141	0.7677497602				
C45	-1.0077253952	-4.1451136815	5.9384883470				
H46	-1.0804558819	-3.2116047407	6.5107816388				
H47	-0.1311989493	-4.6867109904	6.3060862040				
H48	-1.8976687778	-4.7371531929	6.1755612209				
C49	-3.3070261533	-3.1358069815	1.5652371451				
H51	-3.0669063434	-2.7146249563	0.5864856485				
C53	-0.2891899977	-0.1938522759	1.9740053603				
H54	-1.2338785894	-0.5344805311	2.4008504248				
C55	0.7675834801	0.1902132282	2.8850571120				
C56	0.6840124102	0.0732513152	4.2851596021				
C57	1.9137297325	0.7653787018	2.2907985280				
C58	1.7295730926	0.5330043462	5.0794436064				
C59	2.9466831097	1.2427763073	3.0974170888				
C60	2.8540630476	1.1195980623	4.4867020925				
H61	3.6621171877	1.4887767031	5.1124601609				
H62	-0.2020798607	-0.3690627331	4.7321288464				
H63	1.6694840873	0.4502442612	6.1609386878				
H64	3.8199068264	1.7063736386	2.6463422440				
C65	2.0838138518	-0.1956861795	-0.0469290091				
C66	1.8926417650	0.8764533907	0.8122478982				
H67	2.2997308662	0.0029798889	-1.0912593179				
H68	1.9391373107	1.8809530612	0.4031401212				
H69	2.3700857034	-1.1709513286	0.3271301757				
C70	2.9336056002	-2.9785768636	2.5186030782				
H71	3.1241230801	-3.3998821172	3.5113776647				
H72	3.8713296865	-3.0460669988	1.9552199621				
H73	2.6877972693	-1.9223616747	2.6473917163				
C73	2.2011825566	-5.2361418707	1.6619237188				
H74	2.3185739939	-5.6881038070	2.6529608708				
H75	1.4406009602	-5.8147985143	1.1278737518				
H76	3.1515598102	-5.3486841749	1.1280680587				
C76	4.0546135053	-2.2534945849	-2.1403603383				
H77	4.6331482323	-2.0908477661	-3.0558124867				
H78	4.0564165093	-1.3192927319	-1.5743566424				
H79	4.5923599385	-3.0055682569	-1.5520772245				
C79	2.7210813008	-4.0477500182	-3.2848448956				
H80	3.2283635440	-3.8549518427	-4.2364498913				
H81	3.2922897654	-4.8140332261	-2.7483943105				
H82	1.7370069128	-4.4637839354	-3.5207267696				
C82	-2.5157187009	0.8060719614	-3.4714718735				
H83	-2.3929982767	1.2663745037	-4.4592175355				
H84	-3.5865003014	0.7948663979	-3.2451466628				